STIC Database Tracking Number: 1741151

TO: Satayanarayana Gudibande Location: REM-3C04&3C18 Art Unit: 1654 Wednesday, November 16, 2005 Case Serial Number: 10/030944	From: Mary Hale Location: Biotech/Chem Library Rem 1D86 Phone: 2-2507 Mary.Hale@uspto.gov

Search Notes

Feel free to contact me if you have any questions.

Note -- results are printed on both sides of printout

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Gudibande
10/0 30944

```
=> fil reg
COST IN U.S. DOLLARS                    SINCE FILE      TOTAL
                                           ENTRY       SESSION
FULL ESTIMATED COST                         0.63        0.63


FILE 'REGISTRY' ENTERED AT 12:08:55 ON 16 NOV 2005
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   15 NOV 2005  HIGHEST RN 868125-94-4
DICTIONARY FILE UPDATES:  15 NOV 2005  HIGHEST RN 868125-94-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

   Please note that search-term pricing does apply when
   conducting SmartSELECT searches.


********************************************************************
*                                                                *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,  *
* effective March 20, 2005.  A new display format, IDERL, is now   *
* available and contains the CA role and document type information. *
*                                                                *
********************************************************************


Structure search iteration limits have been increased.  See HELP SLIMITS
for details.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=> e rgdldalrggg/sqep
E1          2      RGDLDALRG/SQEP
E2          1      RGDLDALRGG/SQEP
E3          2 -->  RGDLDALRGGG/SQEP
E4          1      RGDLDALRGGGG/SQEP
E5          1      RGDLDALRGGGGG/SQEP
E6          1      RGDLDALRGGGGGG/SQEP
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E8          1      RGDLDGLR/SQEP
E9          2      RGDLDGLRGGG/SQEP
E10         6      RGDLDSLR/SQEP
E11         1      RGDLEPLAARVAGR/SQEP
E12         1      RGDLFAVDTC/SQEP

=> s e3
            2 RGDLDALRGGG/SQEP
        85211 SQL=11
L1          2 (RGDLDALRGGG)/SQEP


Prepared by: Mary Hale @2-2507 Rem Bldg 1D86
```

(RGDLDALRGGG/SQEP AND SQL=11)

=> d 1-2 sqide can

L1   ANSWER 1 OF 2   REGISTRY   COPYRIGHT 2005 ACS on STN
RN   317366-74-8   REGISTRY
CN   Cyclo(L-alanyl-L-leucyl-L-arginylglycylglycylglycyl-L-arginylglycyl-L-
      α-aspartyl-L-leucyl-L-α-aspartyl) (9CI)   (CA INDEX NAME)
FS   PROTEIN SEQUENCE; STEREOSEARCH
SQL   11
NTE   cyclic

SEQ   1 ALRGGGRGDL D
            ========== =
HITS AT: 1-6, 7-11

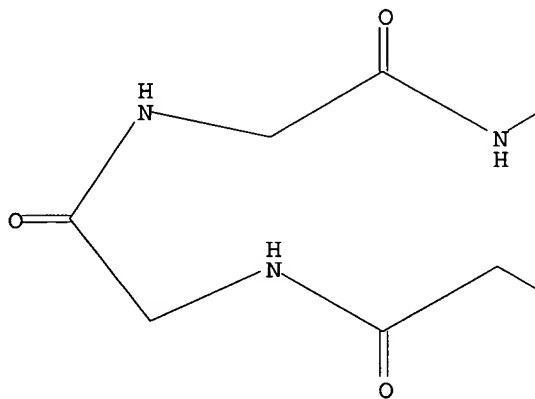**RELATED SEQUENCES AVAILABLE WITH SEQLINK**
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SR   CA
LC   STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES
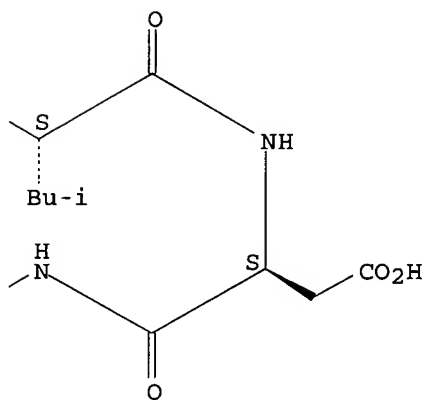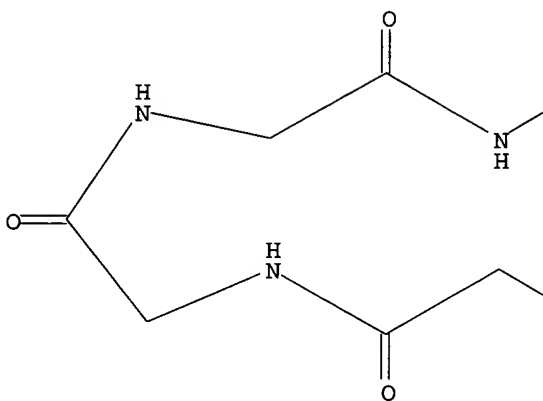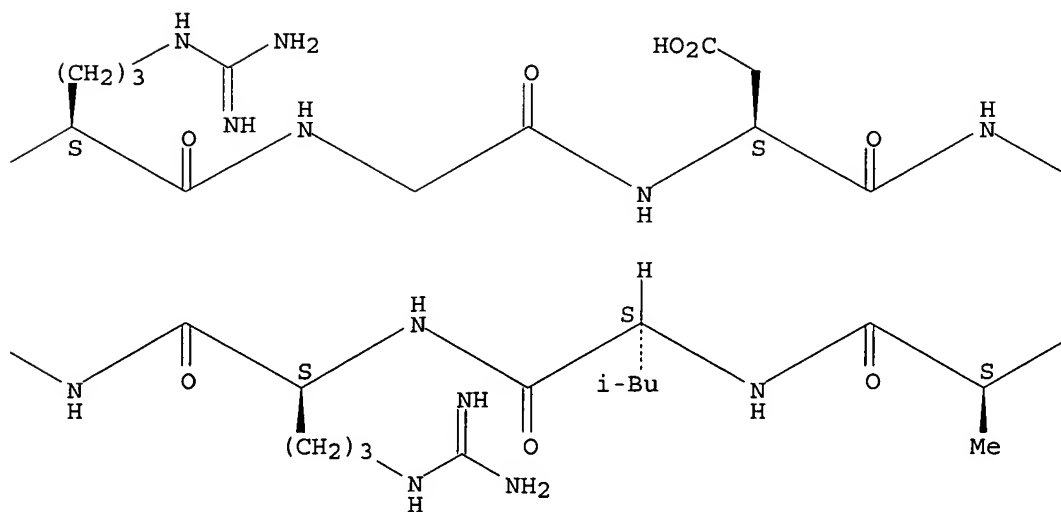   (Uses)

Absolute stereochemistry.

                                             PAGE 1-A

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE   1: 134:86549

L1   ANSWER 2 OF 2   REGISTRY   COPYRIGHT 2005 ACS on STN
RN   317366-58-8   REGISTRY
CN   Cyclo(L-alanyl-L-leucyl-L-arginylglycylglycylglycyl-L-arginylglycyl-L-
     α-aspartyl-L-leucyl-D-α-aspartyl) (9CI)   (CA INDEX NAME)
FS   PROTEIN SEQUENCE; STEREOSEARCH
SQL 11
NTE cyclic

SEQ   1 ALRGGGRGDL D

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

```
  ========== =
HITS AT:   1-6, 7-11
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RELATED SEQUENCES AVAILABLE WITH SEQLINK
MF   C43 H73 N17 O15
SR   CA
LC   STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P   Roles from patents: BIOL (Biological study); PREP (Preparation); USES
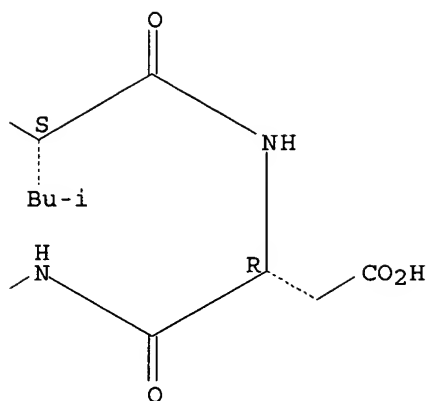   (Uses)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

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                1 REFERENCES IN FILE CA (1907 TO DATE)
                1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE    1:  134:86549


=> fil medl,biosis,embase,caplus;s l1
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                                                ENTRY          SESSION
FULL ESTIMATED COST                             20.47           21.10

FILE 'MEDLINE' ENTERED AT 12:09:57 ON 16 NOV 2005

FILE 'BIOSIS' ENTERED AT 12:09:57 ON 16 NOV 2005
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L2          0 FILE MEDLINE
L3          0 FILE BIOSIS
L4          0 FILE EMBASE
L5          1 FILE CAPLUS

TOTAL FOR ALL FILES
L6          1 L1

=> d ibib abs hitstr

L6    ANSWER 1 OF 1  CAPLUS  COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER:        2001:45035  CAPLUS
DOCUMENT NUMBER:        134:86549
TITLE:                  Preparation of cyclic peptides for use as inhibitors
```

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

```
                              of integrin αvβ6
INVENTOR(S):                  Jonczyk, Alfred; Diefenbach, Beate; Goodman, Simon
PATENT ASSIGNEE(S):           Merck Patent G.m.b.H., Germany
SOURCE:                       Ger. Offen., 20 pp.
                              CODEN: GWXXBX
DOCUMENT TYPE:                Patent
LANGUAGE:                     German
FAMILY ACC. NUM. COUNT:       1
PATENT INFORMATION:
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PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19933173	A1	20010118	DE 1999-19933173	19990715
CA 2379022	AA	20010125	CA 2000-2379022	20000703
WO 2001005810	A2	20010125	WO 2000-EP6188	20000703
WO 2001005810	A3	20010517		

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            W:  AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU,
                CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL,
                IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA,
                MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI,
                SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM,
                AZ, BY, KG, KZ, MD, RU, TJ, TM
            RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
                DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ,
                CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
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| BR 2000012418 | A | 20020326 | BR 2000-12418 | 20000703 |
| EP 1196433 | A2 | 20020417 | EP 2000-943971 | 20000703 |

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JP 2003505395	T2	20030212	JP 2001-511467	20000703
AU 772782	B2	20040506	AU 2000-58236	20000703
NO 2002000176	A	20020114	NO 2002-176	20020114
ZA 2002001275	A	20030822	ZA 2002-1275	20020214

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PRIORITY APPLN. INFO.:                      DE 1999-19933173   A  19990715
                                            WO 2000-EP6188     W  20000703
OTHER SOURCE(S):           MARPAT 134:86549
AB    Title compds. cyclo(Arg-X1-Asp-X2-X3-X4-X5-X6-R1) [(I); X1 = Ser, Gly,
      Thr; X2 = Leu, Ile, Nle, Val, Phe; X3 = Asp, Glu, Lys, Phe; X4 = Gly, Ala,
      Ser; X5 = Leu, Ile, Nle, Val, Phe; X6 = Arg, Har, Lys; R1 = absent, one or
      more ω-amino-carboxy acid residues; all amino acids may be either D-
      or L-configuration] were prepared using solid-phase peptide synthesis and
      tested for activity as integrin αvβ6 inhibitors for therapeutic
      use.  Thus thirty-three I compds. were synthesized on chlorotrityl-
      polystyrol resin and tested for their binding capacities with the
      αvβ6 fibronectin receptor.  Q-values for the tests (Q = IC50
      I/IC50 reference peptide) (reference peptide =
Ac-Arg-Thr-Asp-Leu-Asp-Ser-Leu-Arg-
      NH2; 75 nM) ranged from 233 to 0.014.
IT    317366-58-8P 317366-74-8P
      RL: BAC (Biological activity or effector, except adverse); BSU (Biological
      study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
      BIOL (Biological study); PREP (Preparation); USES (Uses)
         (preparation of cyclic peptides for use as inhibitors of integrin
         αvβ6 in treatment of)
RN    317366-58-8  CAPLUS
CN    Cyclo(L-alanyl-L-leucyl-L-arginylglycylglycylglycyl-L-arginylglycyl-L-
      α-aspartyl-L-leucyl-D-α-aspartyl) (9CI)   (CA INDEX NAME)


Absolute stereochemistry.



Prepared by: Mary Hale @2-2507 Rem Bldg 1D86
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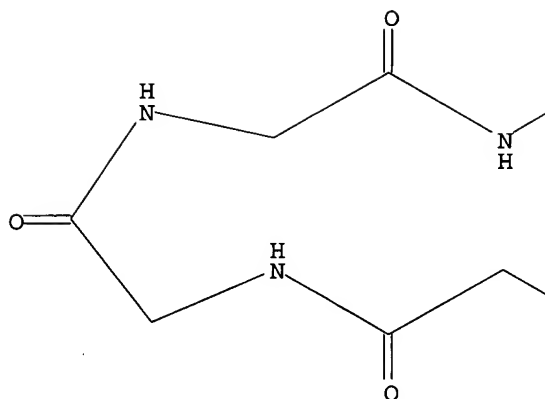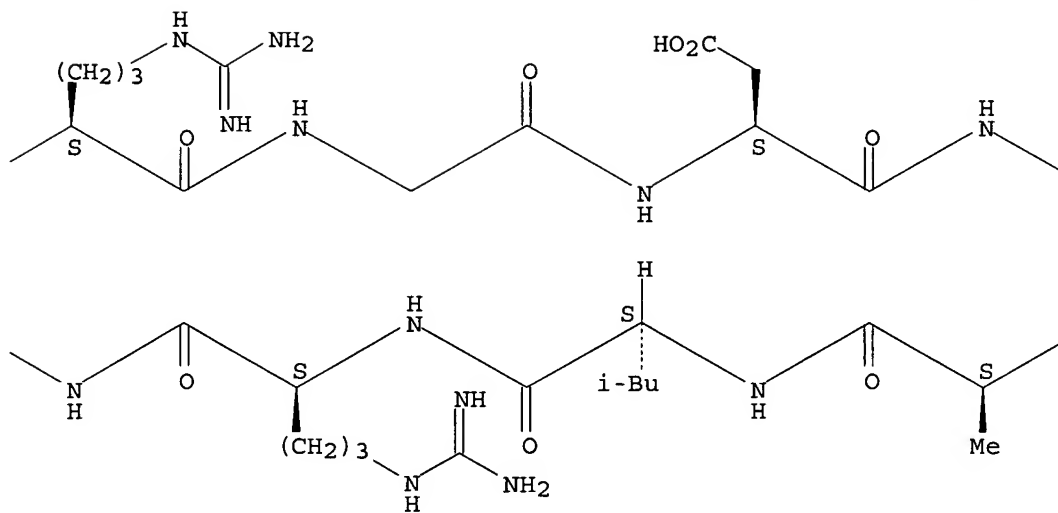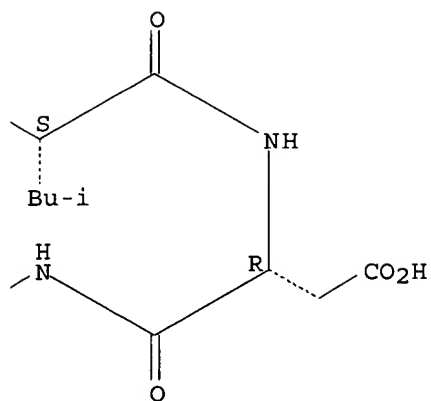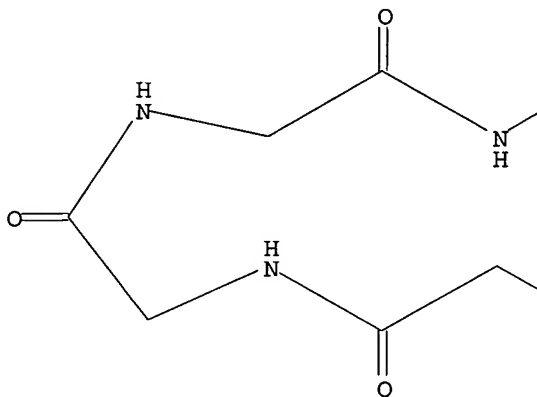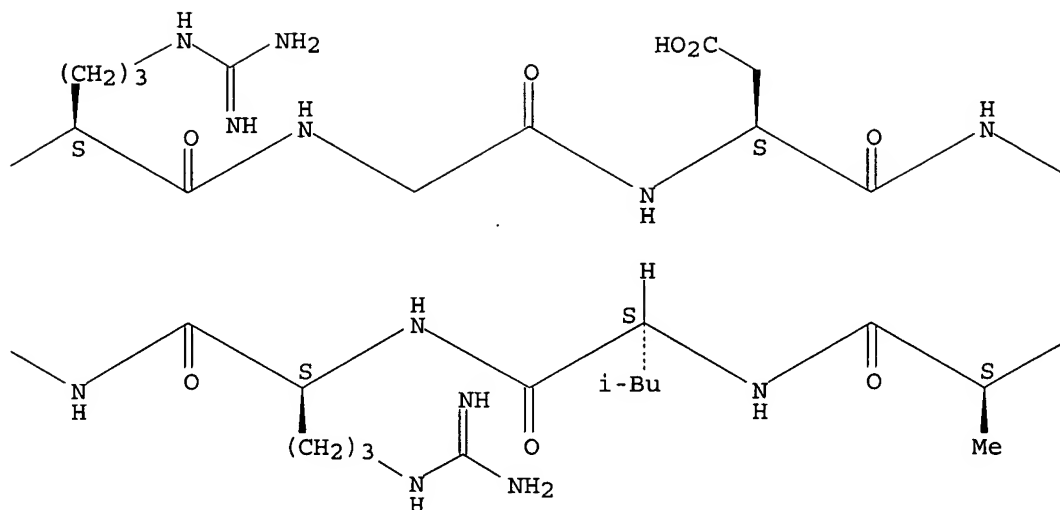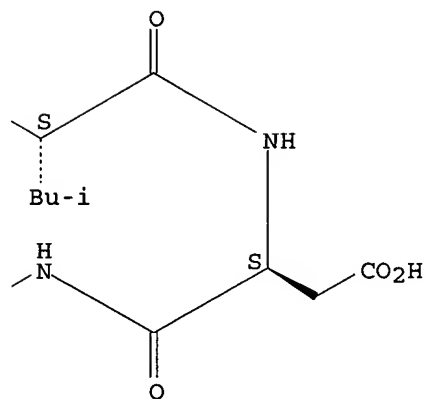
PAGE 1-A

PAGE 1-B

Page 8

PAGE 1-C

RN   317366-74-8   CAPLUS
CN   Cyclo(L-alanyl-L-leucyl-L-arginylglycylglycylglycyl-L-arginylglycyl-L-
      α-aspartyl-L-leucyl-L-α-aspartyl) (9CI)   (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

PAGE 1-B

PAGE 1-C


```
=> fil reg
COST IN U.S. DOLLARS                              SINCE FILE      TOTAL
                                                     ENTRY       SESSION
FULL ESTIMATED COST                                   8.06         29.16

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)        SINCE FILE      TOTAL
                                                     ENTRY       SESSION
CA SUBSCRIBER PRICE                                  -0.73         -0.73
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FILE 'REGISTRY' ENTERED AT 12:10:19 ON 16 NOV 2005
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Property values tagged with IC are from the ZIC/VINITI data file
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STRUCTURE FILE UPDATES: 15 NOV 2005   HIGHEST RN 868125-94-4
DICTIONARY FILE UPDATES: 15 NOV 2005   HIGHEST RN 868125-94-4

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TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

   Please note that search-term pricing does apply when
   conducting SmartSELECT searches.

```
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*                                                              *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,   *
* effective March 20, 2005.  A new display format, IDERL, is now    *
* available and contains the CA role and document type information. *
*                                                              *
****************************************************************
```

Structure search iteration limits have been increased. See HELP SLIMITS
for details.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

```
=> s r[sgt]d[lixvf][dekf][gas][lixvf][rxk]/sqsp
L7          294 R[SGT]D[LIXVF][DEKF][GAS][LIXVF][RXK]/SQSP

=> s l7(l)(cyclo or cyclic)
        3747558 CYCLO
             38 CYCLOS
        3747558 CYCLO
                   (CYCLO OR CYCLOS)
          94190 CYCLIC
L8            0 L7(L)(CYCLO OR CYCLIC)

=> s l7(l)(d or l)
        7686897 D
        1934043 L
L9            0 L7(L)(D OR L)

=> e rgdldglrggg/sqep 5
E1          1       RGDLDAVKGIPFYKGSRA/SQEP
E2          1       RGDLDGLR/SQEP
E3          2 --> RGDLDGLRGGG/SQEP
E4          6       RGDLDSLR/SQEP
E5          1       RGDLEPLAARVAGR/SQEP

=> s e3;e rgdlaalrggg/sqep 5
            2 RGDLDGLRGGG/SQEP
        85211 SQL=11
```

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

```
L10              2 (RGDLDGLRGGG)/SQEP
                   (RGDLDGLRGGG/SQEP AND SQL=11)


E1               1      RGDLAAIVQRLSNRL/SQEP
E2               1      RGDLAAIVQRLSNRLC/SQEP
E3               1 --> RGDLAALRGGG/SQEP
E4               1      RGDLAALSAPPV/SQEP
E5               1      RGDLAFRDDSIWPQEEPAIRPRSSQRVLPMGIQHSKELNRTCCLNGGACMLESFCACPPS
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                        SRTPELPPS/SQEP

=> s e3;e rtdldalrggg/sqep 5
                 1 RGDLAALRGGG/SQEP
             85211 SQL=11
L11              1 (RGDLAALRGGG)/SQEP
                   (RGDLAALRGGG/SQEP AND SQL=11)


E1               2      RTDLDALR'OAA'/SQEP
E2               2      RTDLDALR'OAA-OAA'/SQEP `
E3               2 --> RTDLDALRGGG/SQEP
E4               2      RTDLDGLR/SQEP
E5               2      RTDLDGLRGGG/SQEP

=> s e3;e rgdldalrxx/sqep 5
                 2 RTDLDALRGGG/SQEP
             85211 SQL=11
L12              2 (RTDLDALRGGG)/SQEP
                   (RTDLDALRGGG/SQEP AND SQL=11)


E1               1      RGDLDALRGGGGG/SQEP
E2               1      RGDLDALRGGGGGG/SQEP
E3               0 --> RGDLDALRXX/SQEP
E4               1      RGDLDAVKGIPFYKGSRA/SQEP
E5               1      RGDLDGLR/SQEP

=> e rgdldalr/sqep 5
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E2               1      RGDLD'BAL'LR/SQEP
E3               2 --> RGDLDALR/SQEP
E4               1      RGDLDALR'BAL-BAL'/SQEP
E5               3      RGDLDALR'OAA'/SQEP

=> s e3
                 2 RGDLDALR/SQEP
             66848 SQL=8
L13              2 (RGDLDALR)/SQEP
                   (RGDLDALR/SQEP AND SQL=8)

=> e rtdldalr/sqep 5
E1               1      RTDLD'BAL'LR/SQEP
E2               1      RTDLD'OAA'LR/SQEP
E3               2 --> RTDLDALR/SQEP
E4               2      RTDLDALR'OAA'/SQEP
E5               2      RTDLDALR'OAA-OAA'/SQEP

=> s e3
                 2 RTDLDALR/SQEP
```

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          66848 SQL=8
L14            2 (RTDLDALR)/SQEP
                 (RTDLDALR/SQEP AND SQL=8)

=> e rtdldalra/sqep 5
E1             2      RTDLDALR'OAA'/SQEP
E2             2      RTDLDALR'OAA-OAA'/SQEP
E3             0 --> RTDLDALRA/SQEP
E4             2      RTDLDALRGGG/SQEP
E5             2      RTDLDGLR/SQEP

=> e rgdldalra/sqep 5
E1             3      RGDLDALR'OAA'/SQEP
E2             1      RGDLDALR'OAA-OAA'/SQEP
E3             0 --> RGDLDALRA/SQEP
E4             2      RGDLDALRG/SQEP
E5             1      RGDLDALRGG/SQEP

=> s l10 or l11 or l12 or l13 or l14
L15            9 L10 OR L11 OR L12 OR L13 OR L14

=> d 1-9 sqide can;fil caplus;s l15

L15  ANSWER 1 OF 9  REGISTRY  COPYRIGHT 2005 ACS on STN
RN   527744-99-6  REGISTRY
CN   L-Argininamide, N2-acetyl-L-arginylglycyl-L-α-aspartyl-L-leucyl-D-
     α-aspartyl-L-alanyl-L-leucyl- (9CI)  (CA INDEX NAME)
FS   PROTEIN SEQUENCE; STEREOSEARCH
SQL  8
NTE  modified
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 type              ------ location ------        description
-----------------------------------------------------------------
terminal mod.    Arg-1           -         N-acetyl
terminal mod.    Arg-8           -         C-terminal amide
-----------------------------------------------------------------

SEQ      1 RGDLDALR
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HITS AT:   1-8
MF   C39 H69 N15 O13
SR   CA
LC   STN Files:   CA, CAPLUS
DT.CA CAplus document type:   Conference
RL.NP Roles from non-patents:  BIOL (Biological study); PREP (Preparation)
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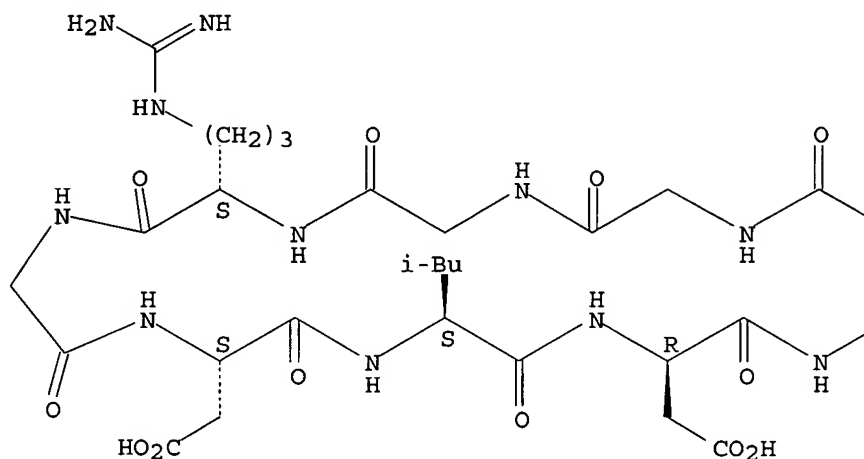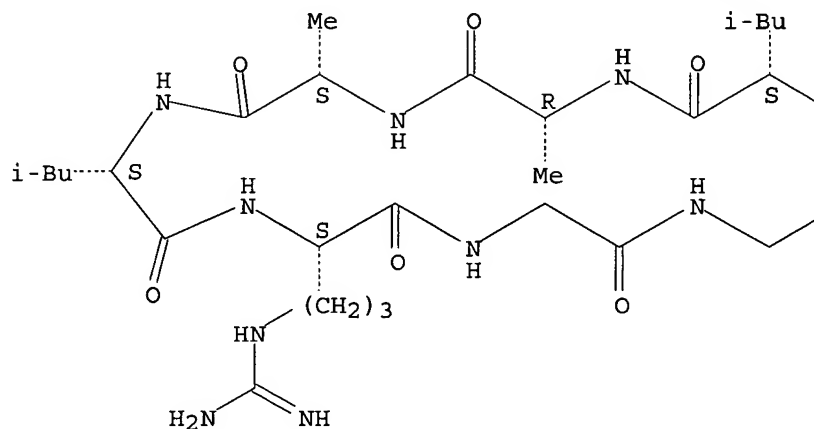
Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE   1: 138:385705

L15 ANSWER 2 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN
RN   317366-75-9 REGISTRY
CN   Cyclo(L-arginylglycyl-L-α-aspartyl-L-leucyl-L-α-aspartylglycyl-
     L-leucyl-L-arginylglycylglycylglycyl) (9CI) (CA INDEX NAME)
FS   PROTEIN SEQUENCE; STEREOSEARCH
SQL **11**
NTE cyclic

SEQ   1 RGDLDGLRGG G
          ========== =
HITS AT: 1-11

RELATED SEQUENCES AVAILABLE WITH SEQLINK
MF   C42 H71 N17 O15

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

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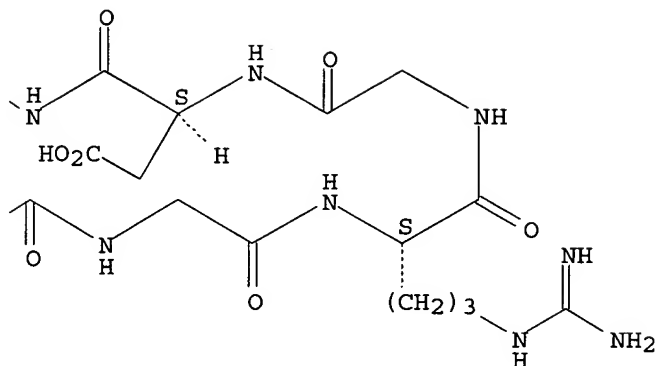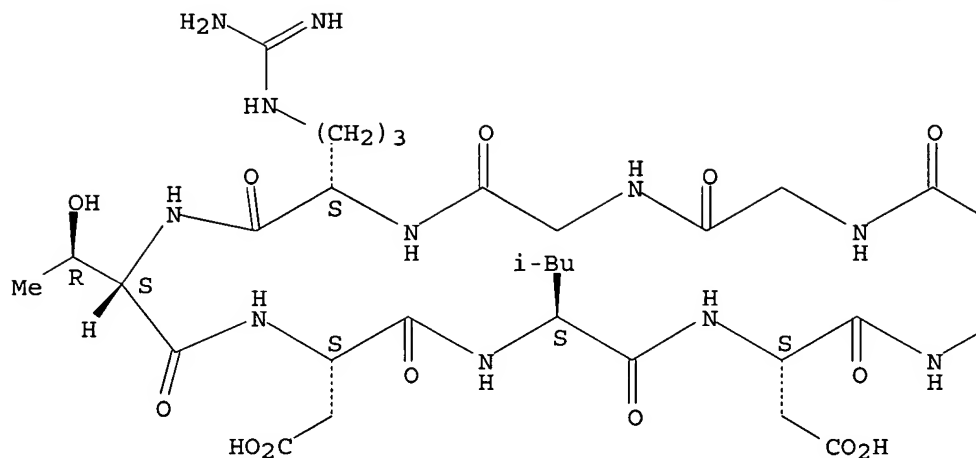LC   STN Files: CA, CAPLUS
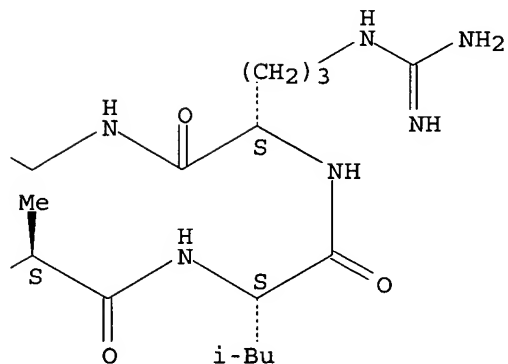DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES
      (Uses)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE   1:   134:86549

L15 ANSWER 3 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN
RN   317366-73-7 REGISTRY
CN   Cyclo(L-arginylglycyl-L-α-aspartyl-L-leucyl-D-α-aspartylglycyl-
     L-leucyl-L-arginylglycylglycylglycyl) (9CI) (CA INDEX NAME)
FS   PROTEIN SEQUENCE; STEREOSEARCH

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

SQL **11**
NTE cyclic

SEQ   1 RGDLDGLRGG G
          ========== =
HITS AT: 1-11

RELATED SEQUENCES AVAILABLE WITH SEQLINK
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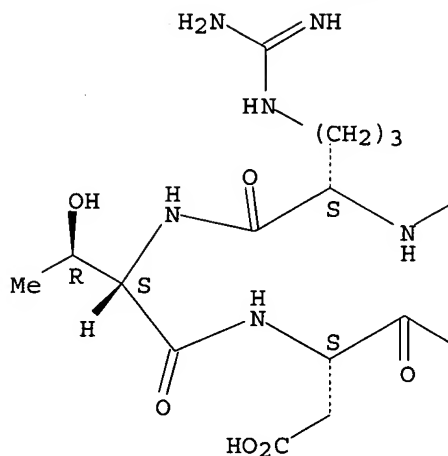SR   CA
LC   STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P   Roles from patents: BIOL (Biological study); PREP (Preparation); USES
       (Uses)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

1 REFERENCES IN FILE CA (1907 TO DATE)

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE   1:   134:86549

L15   ANSWER 4 OF 9   REGISTRY   COPYRIGHT 2005 ACS on STN
RN   317366-67-9   REGISTRY
CN   Cyclo(D-alanyl-L-alanyl-L-leucyl-L-arginylglycylglycylglycyl-L-
       arginylglycyl-L-α-aspartyl-L-leucyl) (9CI)   (CA INDEX NAME)
FS   PROTEIN SEQUENCE; STEREOSEARCH
SQL   **11**
NTE   cyclic

SEQ   1 AALRGGGRGD L
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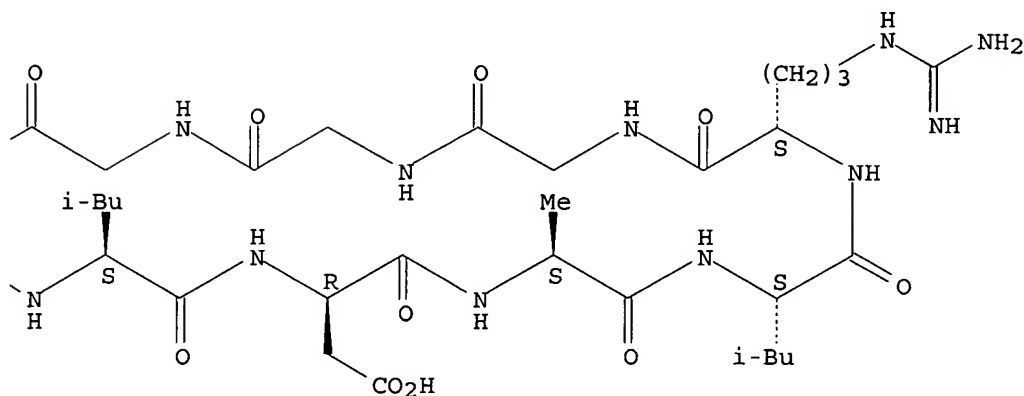DT.CA CAplus document type: Patent
RL.P   Roles from patents: BIOL (Biological study); PREP (Preparation); USES
       (Uses)

Absolute stereochemistry.

PAGE 1-A

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          1 REFERENCES IN FILE CA (1907 TO DATE)
          1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE    1:  134:86549

L15   ANSWER 5 OF 9   REGISTRY   COPYRIGHT 2005 ACS on STN
RN    317366-63-5   REGISTRY
CN    Cyclo(L-alanyl-L-leucyl-L-arginylglycylglycylglycyl-L-arginyl-L-threonyl-L-
      α-aspartyl-L-leucyl-L-α-aspartyl) (9CI)   (CA INDEX NAME)
FS    PROTEIN SEQUENCE; STEREOSEARCH
SQL   11
NTE   cyclic

SEQ      1 ALRGGGRTDL D
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HITS AT:   1-6, 7-11

**RELATED SEQUENCES AVAILABLE WITH SEQLINK**
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SR    CA
LC    STN Files:   CA, CAPLUS
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RL.P  Roles from patents:   BIOL (Biological study); PREP (Preparation); USES
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Absolute stereochemistry.
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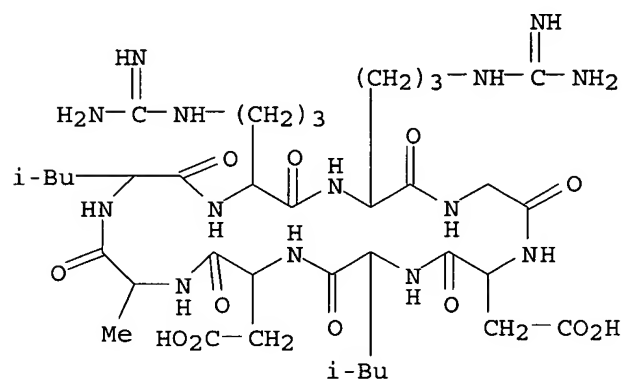
Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

PAGE 1-A

H2N NH

HN

(CH2)3

OH

Me

i-Bu

HO2C

CO2H

PAGE 1-B

H N NH2

(CH2)3
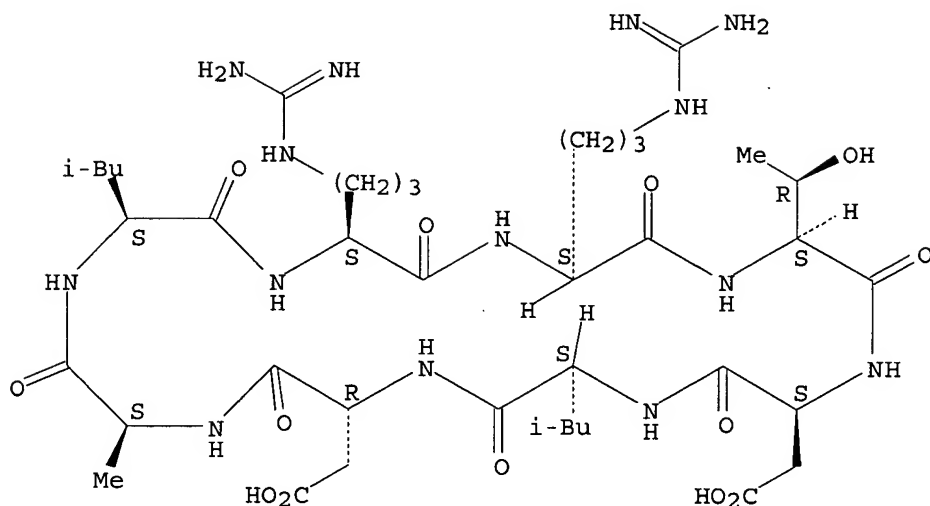
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i-Bu

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1 REFERENCES IN FILE CA (1907 TO DATE)
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REFERENCE   1: 134:86549

L15   ANSWER 6 OF 9   REGISTRY   COPYRIGHT 2005 ACS on STN
RN   317366-61-3   REGISTRY
CN   Cyclo(L-alanyl-L-leucyl-L-arginylglycylglycylglycyl-L-arginyl-L-threonyl-L-
      α-aspartyl-L-leucyl-D-α-aspartyl) (9CI)   (CA INDEX NAME)
FS   PROTEIN SEQUENCE; STEREOSEARCH
SQL   11
NTE   cyclic

SEQ   1 ALRGGGRTDL D
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HITS AT: 1-6, 7-11

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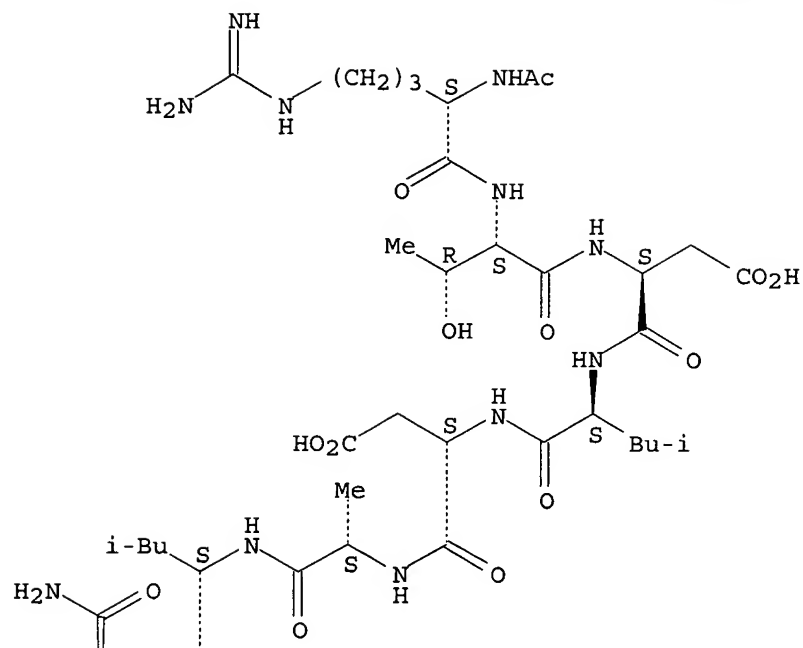MF   C45 H77 N17 O16
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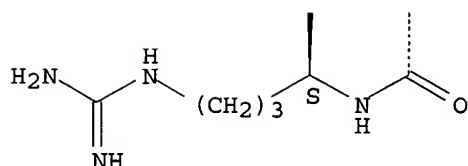DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES
      (Uses)

Absolute stereochemistry.

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PAGE 1-B

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE   1: 134:86549

L15 ANSWER 7 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN
RN   317366-53-3 REGISTRY

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

CN   Cyclo(L-alanyl-L-leucyl-L-arginyl-L-arginylglycyl-L-α-aspartyl-L-
      leucyl-D-α-aspartyl) (9CI)   (CA INDEX NAME)
FS   PROTEIN SEQUENCE; STEREOSEARCH
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NTE   cyclic

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DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES
      (Uses)

          1 REFERENCES IN FILE CA (1907 TO DATE)
          1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE   1: 134:86549

L15   ANSWER 8 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN
RN   317366-50-0 REGISTRY
CN   Cyclo(L-alanyl-L-leucyl-L-arginyl-L-arginyl-L-threonyl-L-α-aspartyl-
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NTE   cyclic

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LC   STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES
      (Uses)

Absolute stereochemistry.

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1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
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REFERENCE   1:   134:86549

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L15   ANSWER 9 OF 9   REGISTRY   COPYRIGHT 2005 ACS on STN
RN    313246-44-5   REGISTRY
CN    L-Argininamide, N2-acetyl-L-arginyl-L-threonyl-L-α-aspartyl-L-leucyl-
      L-α-aspartyl-L-alanyl-L-leucyl- (9CI)   (CA INDEX NAME)
FS    PROTEIN SEQUENCE; STEREOSEARCH
SQL   8
NTE   modified
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terminal mod.    Arg-8            -           C-terminal amide
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SEQ      1 RTDLDALR
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HITS AT:    1-8
MF    C41 H73 N15 O14
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LC    STN Files:   CA, CAPLUS
DT.CA  CAplus document type:  Patent
RL.P   Roles from patents:  BIOL (Biological study); PREP (Preparation); USES
       (Uses)
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Absolute stereochemistry.

1 REFERENCES IN FILE CA (1907 TO DATE)
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REFERENCE   1:   134:42449

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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-0.73

FILE 'CAPLUS' ENTERED AT 12:16:33 ON 16 NOV 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

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FILE COVERS 1907 - 16 Nov 2005   VOL 143 ISS 21
FILE LAST UPDATED: 15 Nov 2005   (20051115/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

L16   3 L15

=> d 1-3 ibib abs hitseq

L16 ANSWER 1 OF 3   CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:692564   CAPLUS
DOCUMENT NUMBER: 138:385705
TITLE: Linear and cyclic peptides for integrin
                         αvβ6 inhibition
AUTHOR(S):   Zischinsky, Gunther; Groth, Ulrich; Diefenbach, Beate;
                         Jonczyk, Alfred
CORPORATE SOURCE: Faculty of Chemistry, University of Konstanz, Germany
SOURCE: Peptides: The Wave of the Future, Proceedings of the
                         Second International and the Seventeenth American
                         Peptide Symposium, San Diego, CA, United States, June
                         9-14, 2001 (2001), 733-734. Editor(s): Lebl, Michal;
                         Houghten, Richard A. American Peptide Society: San
                         Diego, Calif.
                         CODEN: 69DBAL; ISBN: 0-9715560-0-8
DOCUMENT TYPE: Conference
LANGUAGE: English
AB   A symposium report. Integrin αvβ6 inhibitory activity of
     peptides was enhanced by cyclization, which increased rigidity and
     proteolytic stability. The best linear derivative was the non-RGD peptide
     Ac-TRDLdSLR-NH2. Selected cyclic peptides proved to be stable in human
     blood plasma with half life-times of more than 30 h.
IT   527744-99-6P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL
     (Biological study); PREP (Preparation)
        (linear and cyclic peptides as inhibitors of integrin αvβ6)
RN   527744-99-6 CAPLUS
CN   L-Argininamide, N2-acetyl-L-arginylglycyl-L-α-aspartyl-L-leucyl-D-
     α-aspartyl-L-alanyl-L-leucyl- (9CI) (CA INDEX NAME)

NTE modified

SEQ   1 RGDLDALR

Absolute stereochemistry.

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86
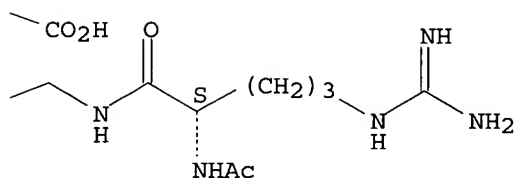
PAGE 1-A

PAGE 1-B

REFERENCE COUNT: 4   THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS
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L16   ANSWER 2 OF 3   CAPLUS   COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:45035   CAPLUS
DOCUMENT NUMBER: 134:86549
TITLE: Preparation of cyclic peptides for use as inhibitors
                         of integrin αvβ6
INVENTOR(S):   Jonczyk, Alfred; Diefenbach, Beate; Goodman, Simon
PATENT ASSIGNEE(S):   Merck Patent G.m.b.H., Germany
SOURCE: Ger. Offen., 20 pp.
                         CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

        PATENT NO.   KIND   DATE   APPLICATION NO.   DATE
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        DE 19933173   A1   20010118   DE 1999-19933173   19990715
        CA 2379022   AA   20010125   CA 2000-2379022   20000703
        WO 2001005810   A2   20010125   WO 2000-EP6188   20000703

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

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        IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA,
        MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI,
        SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM,
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EP 1196433           A2      20020417    EP 2000-943971         20000703
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AU 772782            B2      20040506    AU 2000-58236          20000703
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ZA 2002001275        A       20030822    ZA 2002-1275           20020214
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PRIORITY APPLN. INFO.:                   DE 1999-19933173   A  19990715
                                         WO 2000-EP6188     W  20000703
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OTHER SOURCE(S):   MARPAT 134:86549

AB   Title compds. cyclo(Arg-X1-Asp-X2-X3-X4-X5-X6-R1) [(I); X1 = Ser, Gly,
      Thr; X2 = Leu, Ile, Nle, Val, Phe; X3 = Asp, Glu, Lys, Phe; X4 = Gly, Ala,
      Ser; X5 = Leu, Ile, Nle, Val, Phe; X6 = Arg, Har, Lys; R1 = absent, one or
      more ω-amino-carboxy acid residues; all amino acids may be either D-
      or L-configuration] were prepared using solid-phase peptide synthesis and
      tested for activity as integrin αvβ6 inhibitors for therapeutic
      use. Thus thirty-three I compds. were synthesized on chlorotrityl-
      polystyrol resin and tested for their binding capacities with the
      αvβ6 fibronectin receptor. Q-values for the tests (Q = IC50
      I/IC50 reference peptide) (reference peptide =
Ac-Arg-Thr-Asp-Leu-Asp-Ser-Leu-Arg-
      NH2; 75 nM) ranged from 233 to 0.014.
IT   **317366-50-0P 317366-53-3P 317366-61-3P**
      317366-63-5P 317366-67-9P 317366-73-7P
      317366-75-9P
      RL: BAC (Biological activity or effector, except adverse); BSU (Biological
      study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
      BIOL (Biological study); PREP (Preparation); USES (Uses)
          (preparation of cyclic peptides for use as inhibitors of integrin
          αvβ6 in treatment of)
RN   317366-50-0 CAPLUS
CN   Cyclo(L-alanyl-L-leucyl-L-arginyl-L-arginyl-L-threonyl-L-α-aspartyl-
      L-leucyl-D-α-aspartyl) (9CI) (CA INDEX NAME)

NTE   cyclic

SEQ   1 ALRRTDLD

Absolute stereochemistry.

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

RN 317366-53-3 CAPLUS
CN Cyclo(L-alanyl-L-leucyl-L-arginyl-L-arginylglycyl-L-α-aspartyl-L-leucyl-D-α-aspartyl) (9CI) (CA INDEX NAME)

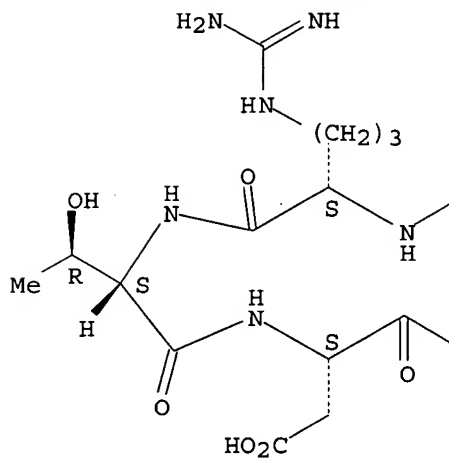NTE cyclic

SEQ 1 ALRRGDLD

RN 317366-61-3 CAPLUS
CN Cyclo(L-alanyl-L-leucyl-L-arginylglycylglycylglycyl-L-arginyl-L-threonyl-L-α-aspartyl-L-leucyl-D-α-aspartyl) (9CI) (CA INDEX NAME)
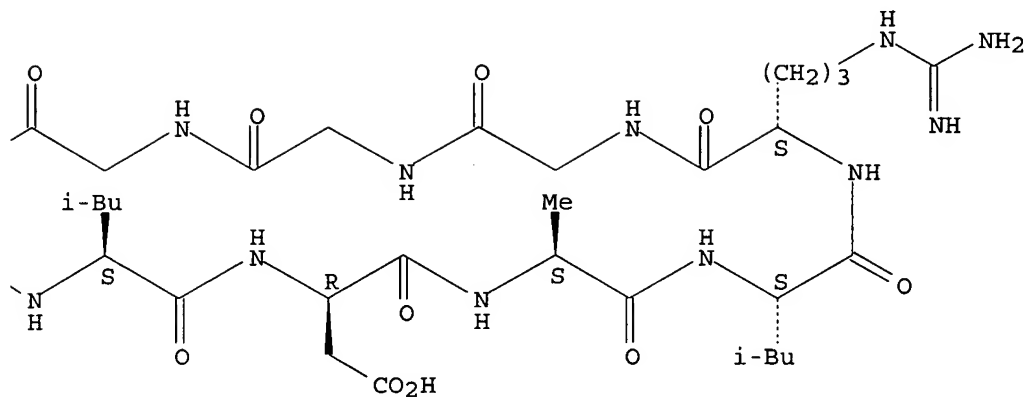
NTE cyclic

SEQ 1 ALRGGGRTDL D

Absolute stereochemistry.
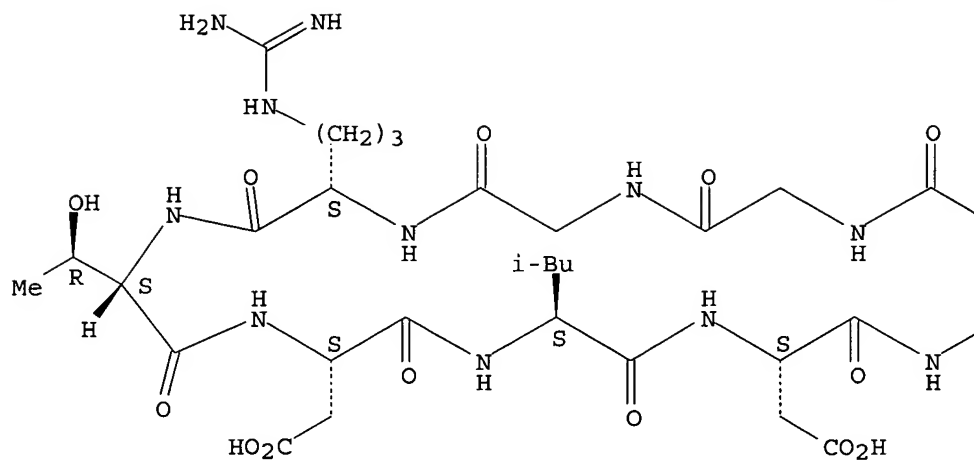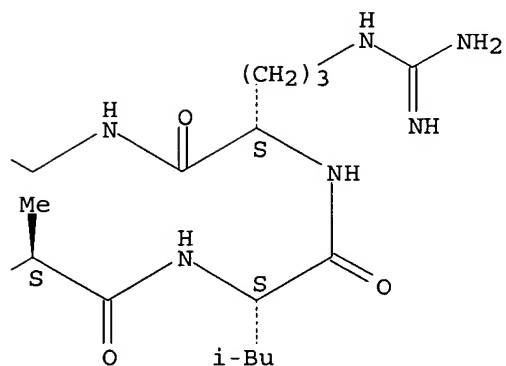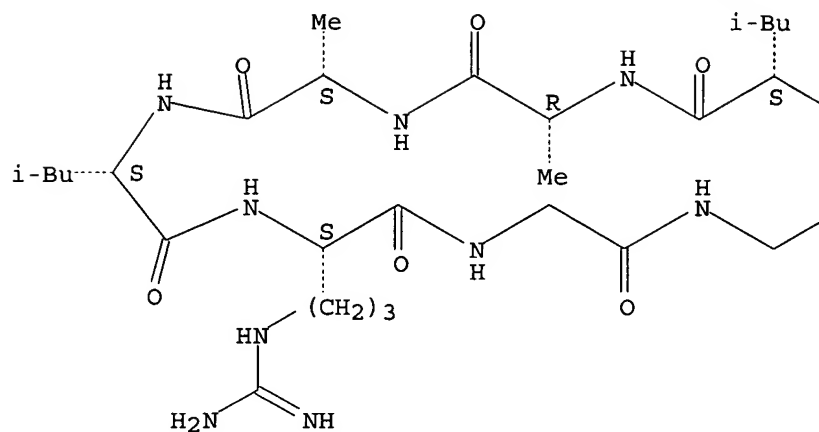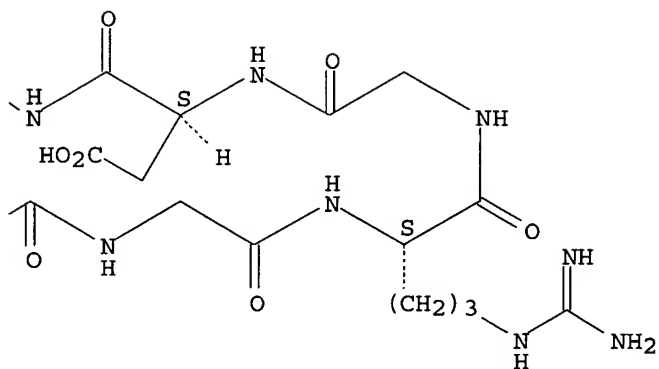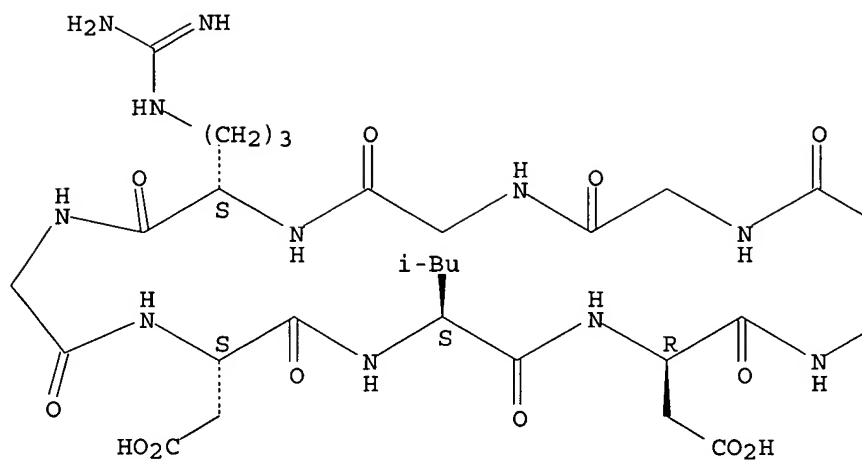
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PAGE 1-B

RN   317366-63-5 CAPLUS
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      α-aspartyl-L-leucyl-L-α-aspartyl) (9CI)   (CA INDEX NAME)

NTE   cyclic

SEQ   1 ALRGGGRTDL D

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

RN   317366-67-9   CAPLUS
CN   Cyclo(D-alanyl-L-alanyl-L-leucyl-L-arginylglycylglycylglycyl-L-
      arginylglycyl-L-α-aspartyl-L-leucyl) (9CI)   (CA INDEX NAME)

NTE   cyclic

SEQ   1 AALRGGGRGD L

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

RN   317366-73-7   CAPLUS
CN   Cyclo(L-arginylglycyl-L-α-aspartyl-L-leucyl-D-α-aspartylglycyl-
      L-leucyl-L-arginylglycylglycylglycyl) (9CI)   (CA INDEX NAME)

NTE   cyclic

SEQ   1 RGDLDGLRGG G

Absolute stereochemistry.

RN   317366-75-9   CAPLUS
CN   Cyclo(L-arginylglycyl-L-α-aspartyl-L-leucyl-L-α-aspartylglycyl-
      L-leucyl-L-arginylglycylglycylglycyl) (9CI)   (CA INDEX NAME)

NTE   cyclic

SEQ   1 RGDLDGLRGG G

Absolute stereochemistry.

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

L16   ANSWER 3 OF 3   CAPLUS   COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2000:909678   CAPLUS
DOCUMENT NUMBER: 134:42449
TITLE: Synthesis of peptide inhibitors of integrin
                         αvβ6
INVENTOR(S):   Jonczyk, Alfred; Diefenbach, Beate; Groth, Ulrich;
                         Zischinsky, Gunther
PATENT ASSIGNEE(S):   Merck Patent G.m.b.H., Germany
SOURCE: Ger. Offen., 34 pp.
                         CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

    PATENT NO.   KIND   DATE   APPLICATION NO.   DATE

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

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DE 19929410            A1    20001228  DE 1999-19929410        19990626
CA 2377224            AA    20010104  CA 2000-2377224         20000613
WO 2001000660         A1    20010104  WO 2000-EP5404          20000613
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        ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU,
        LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD,
        SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU,
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    RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
        DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ,
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JP 2003503422         T2    20030128  JP 2001-507066          20000613
AU 771099             B2    20040311  AU 2000-62630           20000613
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ZA 2002000673         A     20030424  ZA 2002-673             20020124
PRIORITY APPLN. INFO.:                DE 1999-19929410      A  19990626
                                      WO 2000-EP5404        W  20000613
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OTHER SOURCE(S):   MARPAT 134:42449

AB   The invention describes the solid-phase synthesis of peptides
      H3CC(O)-Arg-X1-Asp-X2-X3-X4-X5-X6-NH2 [(I); X1 = Ser, Gly, Thr, Asp, Arg,
      Val, Tyr, His or Ala; X2 = Leu, Ile, Nle, Val or Phe; X3 = Asp, Glu, Lys,
      Phe, Aib, Nal, Gly, Ala, Bgl or Phg; X4 = Gly, Ala, Ser, βAla or
      ωAbu; X5 = Leu, Ile, Nle, Val, Phe; X6 = Arg, Har, Lys, Leu, Orn,
      Phe, Ala, Tyr, Gly, Ser or Asp] for use as inhibitors of αvβ6
      integrin in the treatment of disease. Thus I [X1 = Gly; X2 = Leu; X3 =
      D-Asp; X4 = Ser; X5 = Leu; X6 = Arg (II)] was synthesized using
      solid-phase techniques. In in vitro binding tests, using peptide
      H3CC(O)-Arg-Thr-Asp-Leu-Asp-Ser-Leu-Arg-NH2 as standard, II had Q-value (IC50
      test peptide/IC50 standard) 0.15 at 75 nM.
IT   **313246-44-5P**
      RL: BAC (Biological activity or effector, except adverse); BSU (Biological
      study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
      BIOL (Biological study); PREP (Preparation); USES (Uses)
         (preparation of peptide inhibitors of integrin αvβ6 for treatment
         of disease)
RN   313246-44-5 CAPLUS
CN   L-Argininamide, N2-acetyl-L-arginyl-L-threonyl-L-α-aspartyl-L-leucyl-
      L-α-aspartyl-L-alanyl-L-leucyl- (9CI) (CA INDEX NAME)

NTE   modified

SEQ   1 RTDLDALR

Absolute stereochemistry.

PAGE 1-A

PAGE 2-A


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Prepared by: Mary Hale @2-2507 Rem Bldg 1D86
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FULL ESTIMATED COST                              28.86     199.89

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CA SUBSCRIBER PRICE                              -2.19      -2.92

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L3           30 L1 AND L2

=> d 1-30 sqide can
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L3   ANSWER 1 OF 30   REGISTRY   COPYRIGHT 2005 ACS on STN
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      arginyl-L-threonyl-L-α-aspartyl-L-leucyl-D-α-aspartyl) (9CI)
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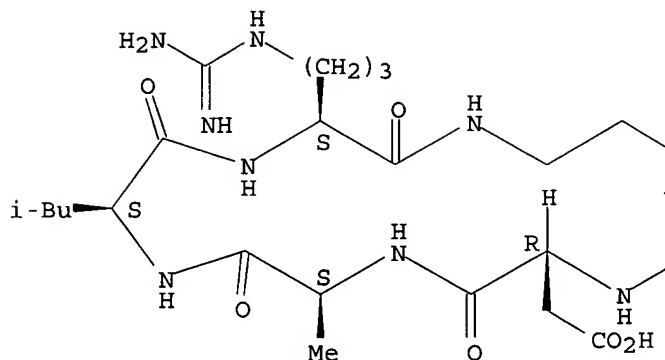MF   C47 H82 N16 O15
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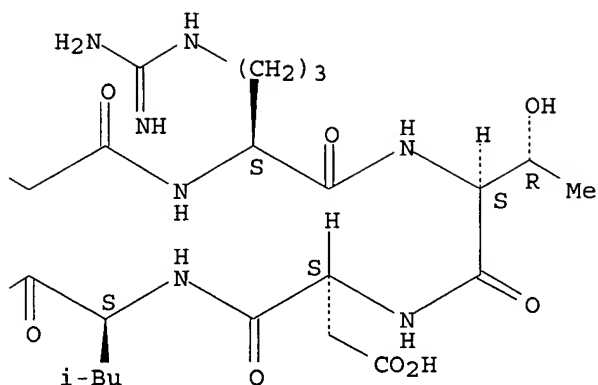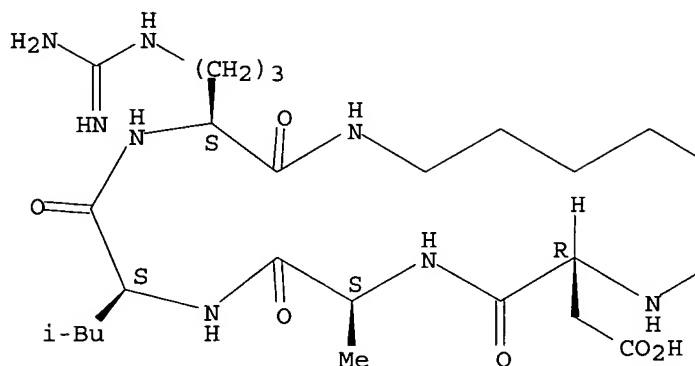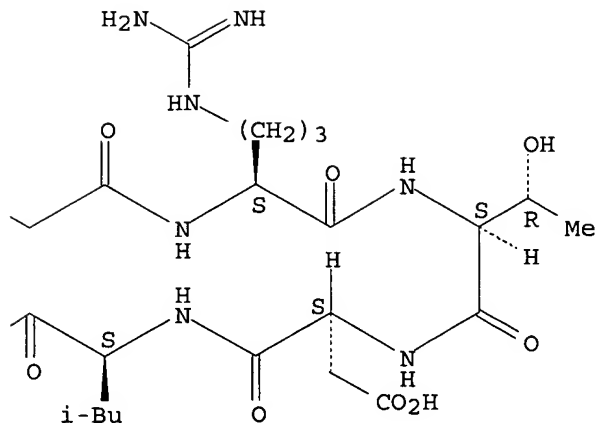RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES
      (Uses)

Absolute stereochemistry.

PAGE 1-A

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                 1 REFERENCES IN FILE CA (1907 TO DATE)
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REFERENCE    1:  134:86549

L3    ANSWER 2 OF 30  REGISTRY  COPYRIGHT 2005 ACS on STN
RN    317366-79-3  REGISTRY
CN    Cyclo(L-alanyl-L-leucyl-L-arginyl-6-aminohexanoyl-6-aminohexanoyl-L-
      arginyl-L-threonyl-L-α-aspartyl-L-leucyl-D-α-aspartyl) (9CI)
      (CA INDEX NAME)
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uncommon           Oaa-5              -           -
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       (Uses)

Absolute stereochemistry.
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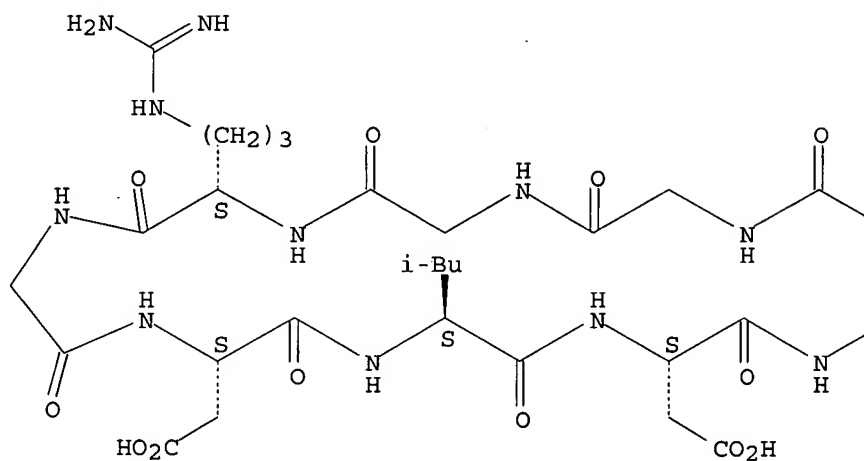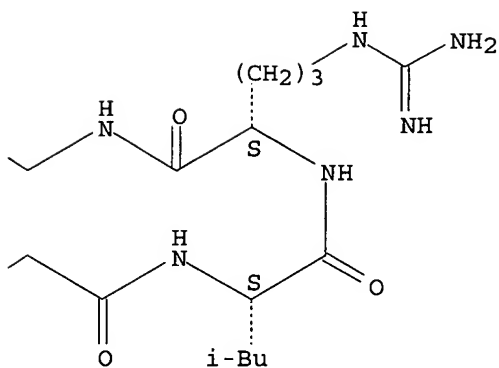
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REFERENCE   1:   134:86549

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CN    Cyclo(L-alanyl-L-leucyl-L-arginyl-4-aminobutanoyl-L-arginylglycyl-L-
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HITS AT:   1-3, 5-9
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Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

RELATED SEQUENCES AVAILABLE WITH SEQLINK
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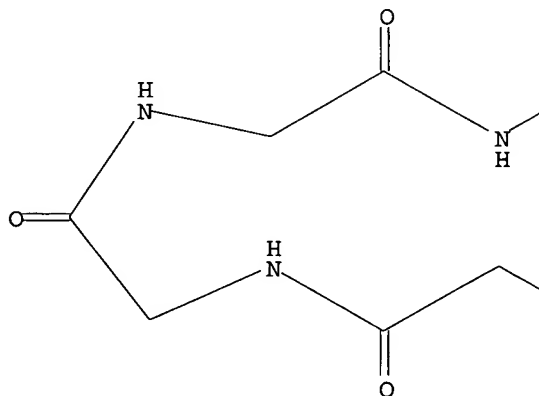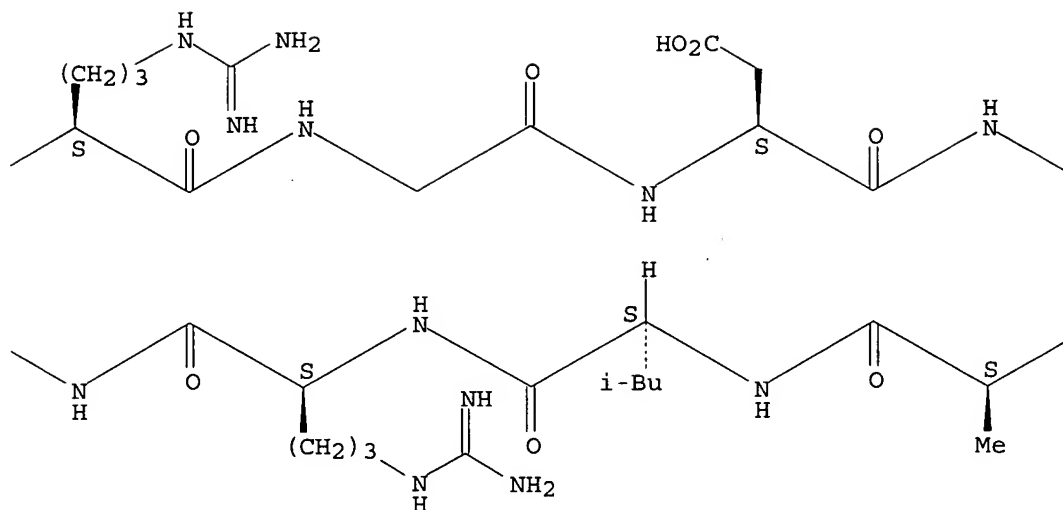


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CN    Cyclo(L-alanyl-L-leucyl-L-arginyl-4-aminobutanoyl-L-arginyl-L-threonyl-L-
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FS    PROTEIN SEQUENCE; STEREOSEARCH
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NTE   cyclic
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uncommon        Oaa-4              -          -
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HITS AT:  1-3, 5-9
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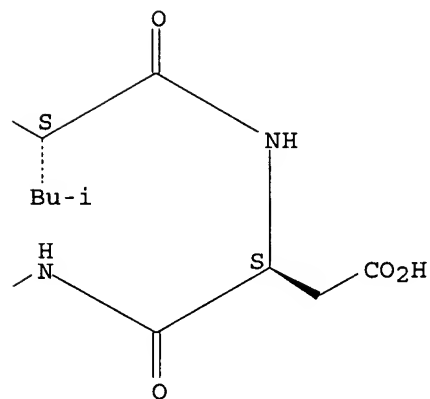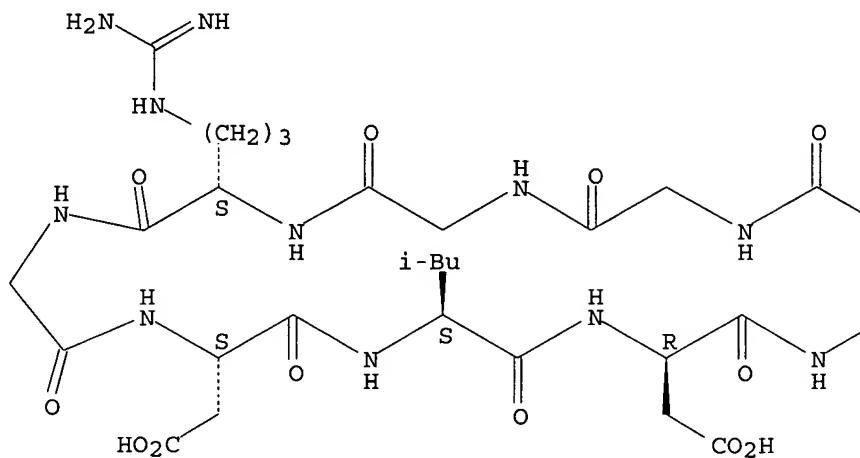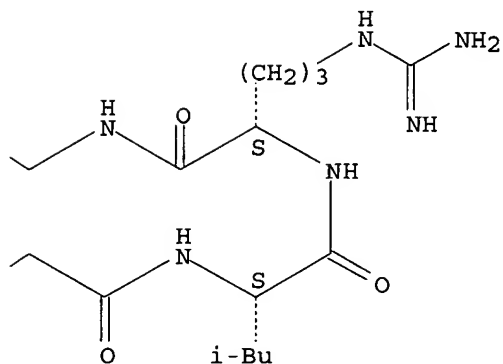
Absolute stereochemistry.

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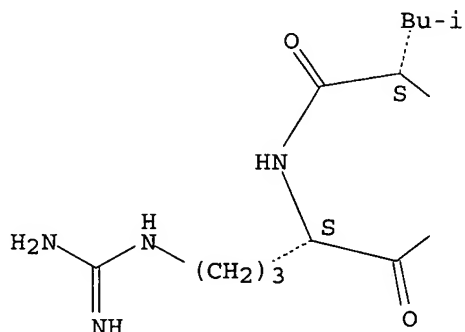1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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NTE   cyclic
-------------------------------------------------------------------------
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-------------------------------------------------------------------------

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HITS AT:   1-3, 5-9
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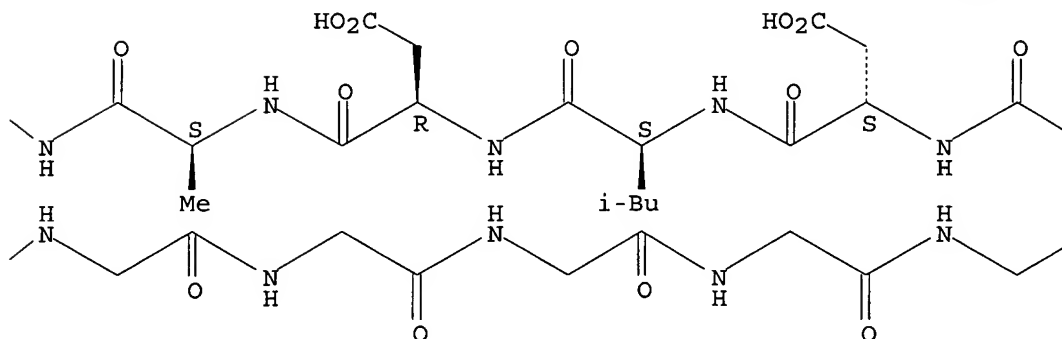
Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

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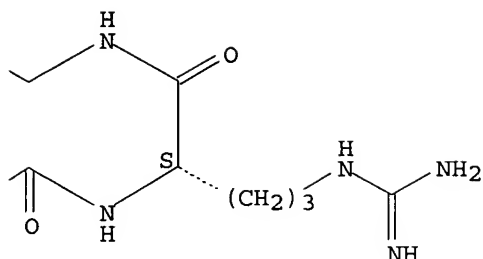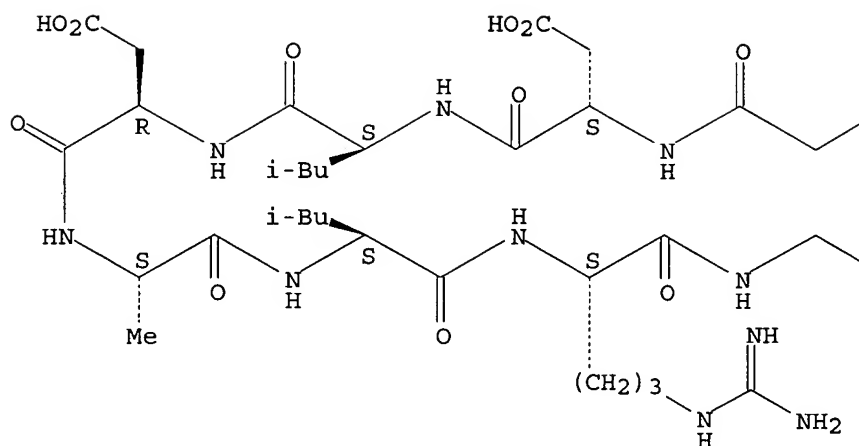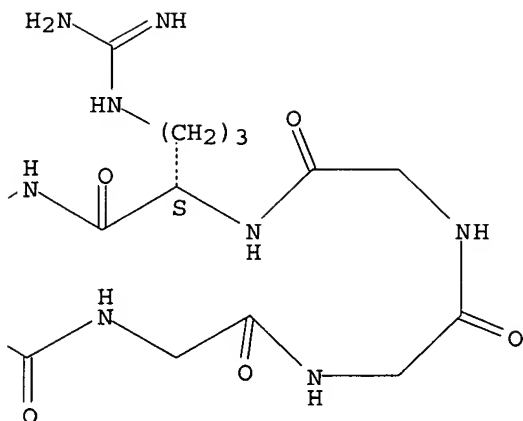
Absolute stereochemistry.

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REFERENCE   1:   134:86549

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CN    Cyclo(L-arginylglycyl-L-α-aspartyl-L-leucyl-L-α-aspartylglycyl-
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FS    PROTEIN SEQUENCE; STEREOSEARCH
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NTE   cyclic

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HITS AT:   1-8
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      (Uses)
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Absolute stereochemistry.

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Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

REFERENCE   1: 134:86549

L3   ANSWER 7 OF 30 REGISTRY COPYRIGHT 2005 ACS on STN
RN   317366-74-8 REGISTRY
CN   Cyclo(L-alanyl-L-leucyl-L-arginylglycylglycylglycyl-L-arginylglycyl-L-
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HITS AT: 1-3, 7-11

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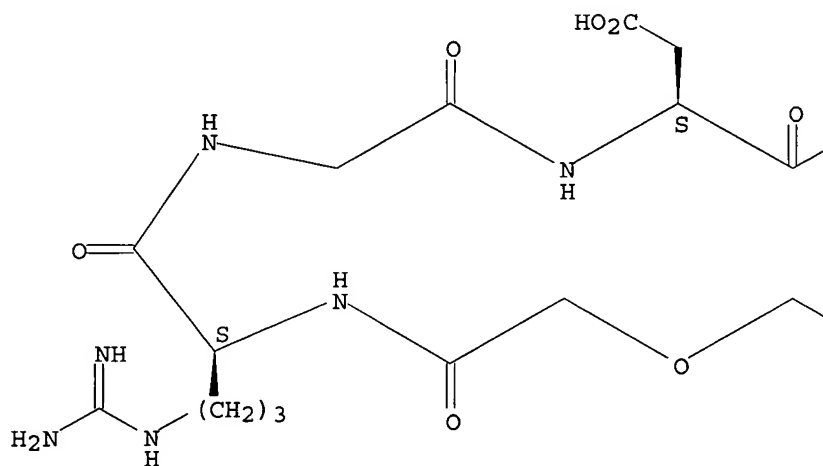MF   C43 H73 N17 O15
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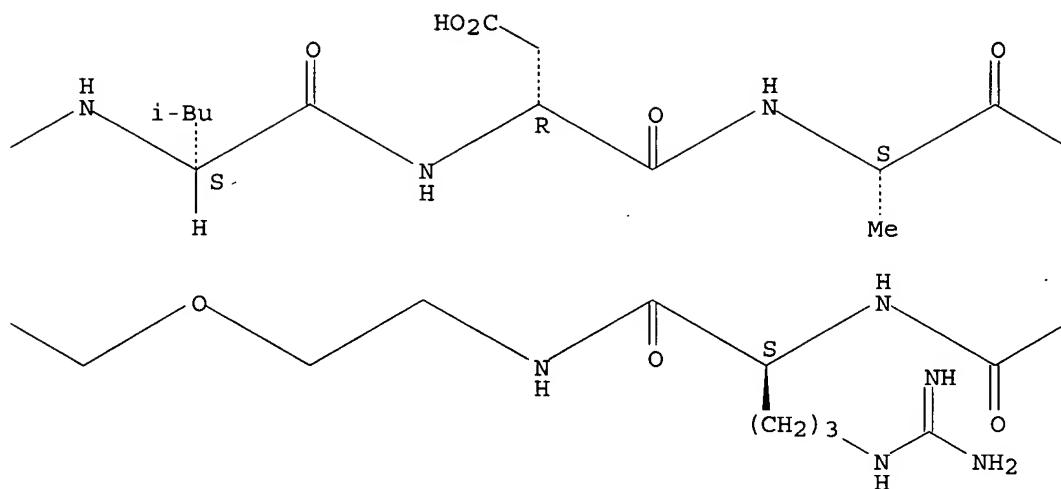LC   STN Files: CA, CAPLUS
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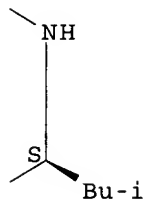   (Uses)

Absolute stereochemistry.

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1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE   1: 134:86549

L3   ANSWER 8 OF 30 REGISTRY COPYRIGHT 2005 ACS on STN
RN   317366-73-7 REGISTRY
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FS   PROTEIN SEQUENCE; STEREOSEARCH
SQL   11
NTE   **cyclic**

SEQ   1 RGDLDGLRGG G

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

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HITS AT:   1-8
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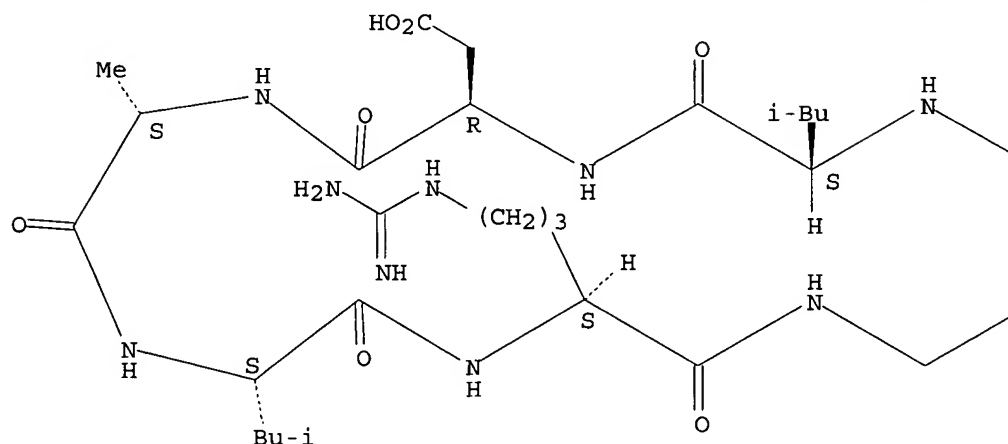```
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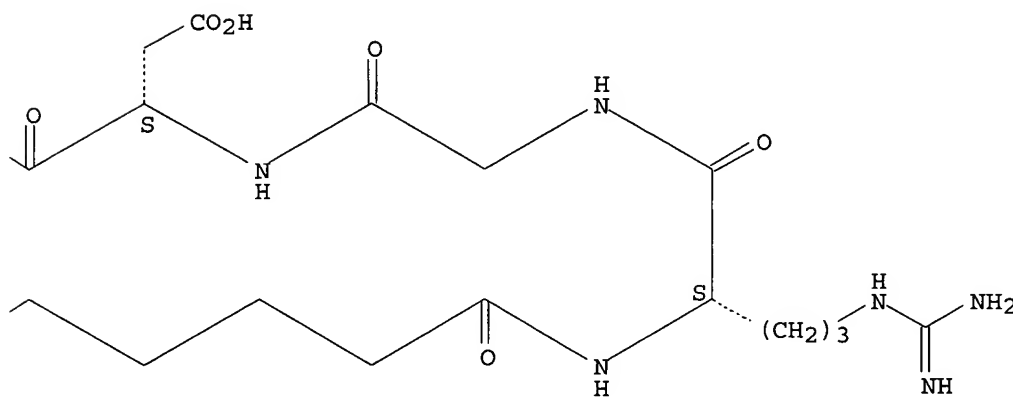
Absolute stereochemistry.

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REFERENCE   1:  134:86549
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Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

L3   ANSWER 9 OF 30 REGISTRY COPYRIGHT 2005 ACS on STN
RN   317366-72-6 REGISTRY
CN   Cyclo(L-alanyl-L-leucyl-L-arginylglycylglycylglycylglycylglycyl-L-
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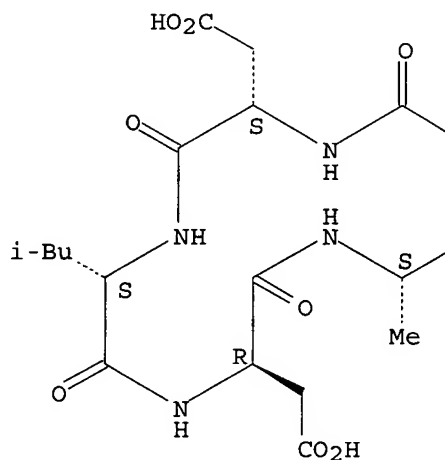MF   C47 H79 N19 O17
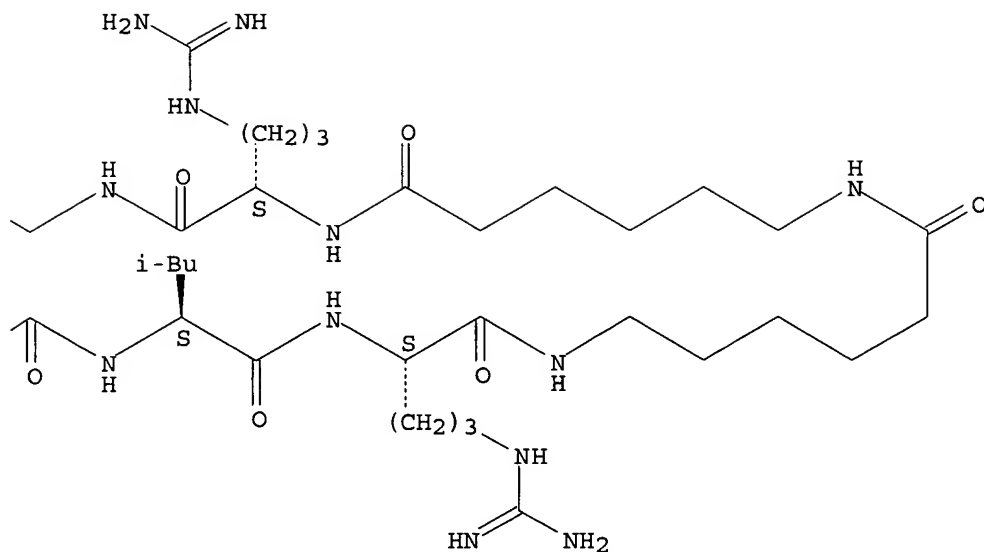SR   CA
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Absolute stereochemistry.

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PAGE 1-B

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REFERENCE   1: 134:86549

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      (Uses)
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Absolute stereochemistry.

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REFERENCE   1:  134:86549

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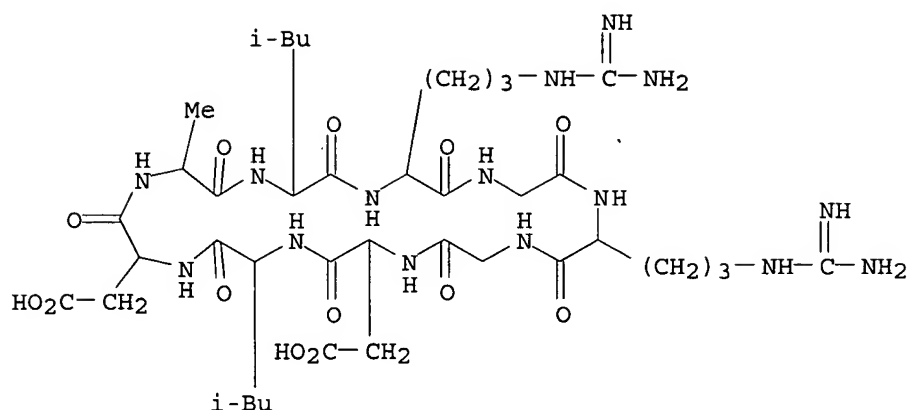
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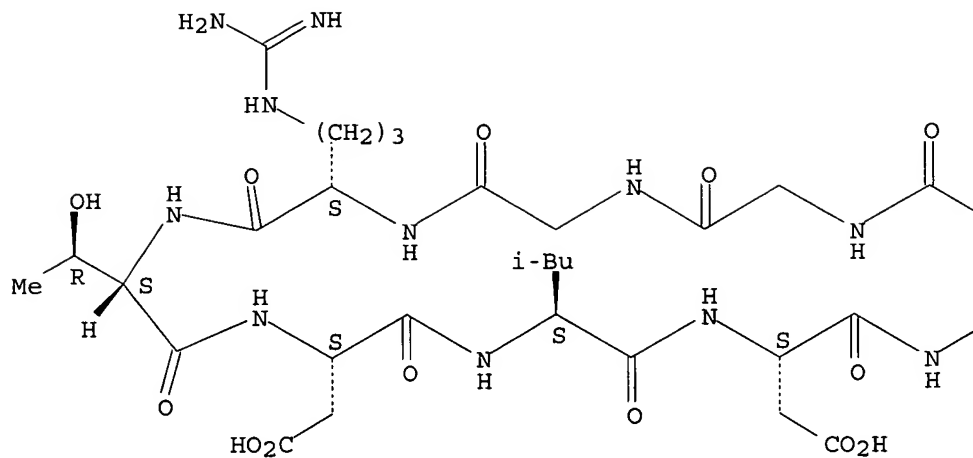
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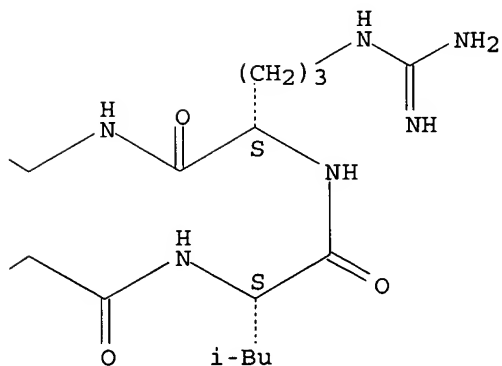**RELATED SEQUENCES AVAILABLE WITH SEQLINK**
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       (Uses)

Absolute stereochemistry.

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REFERENCE   1:   134:86549

L3   ANSWER 12 OF 30 REGISTRY   COPYRIGHT 2005 ACS on STN
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NTE   **cyclic**
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 type   ------ location ------   description
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uncommon   Oaa-4   -   -

SEQ   1 ALRXRGDLD
           === =====

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

HITS AT: 1-3, 5-9

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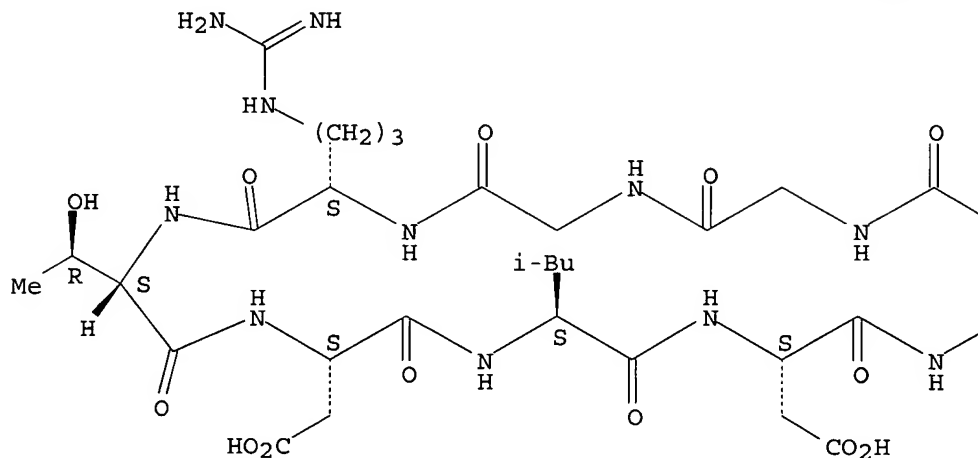SR   CA
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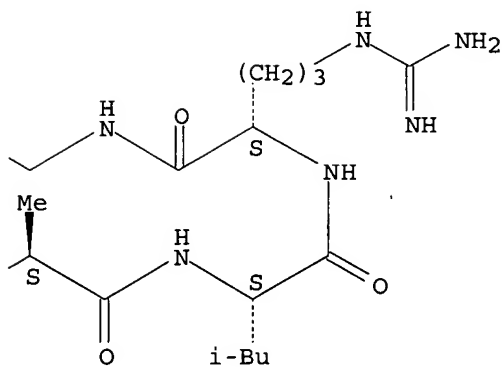DT.CA CAplus document type: Patent
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Absolute stereochemistry.

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1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE   1: 134:86549

L3   ANSWER 13 OF 30   REGISTRY   COPYRIGHT 2005 ACS on STN
RN   317366-68-0   REGISTRY
CN   Cyclo(L-alanyl-L-leucyl-L-arginyl-6-aminohexanoyl-6-aminohexanoyl-L-

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

arginylglycyl-L-α-aspartyl-L-leucyl-D-α-aspartyl) (9CI)   (CA
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FS   PROTEIN SEQUENCE; STEREOSEARCH
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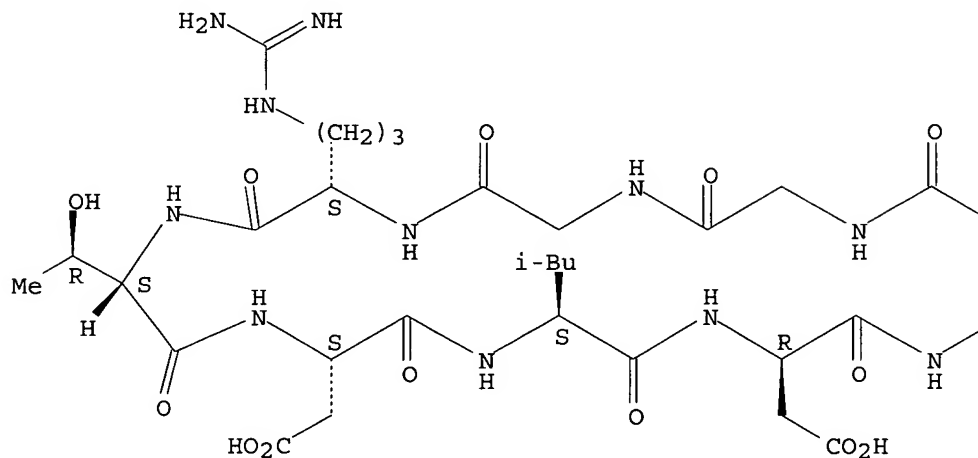SR   CA
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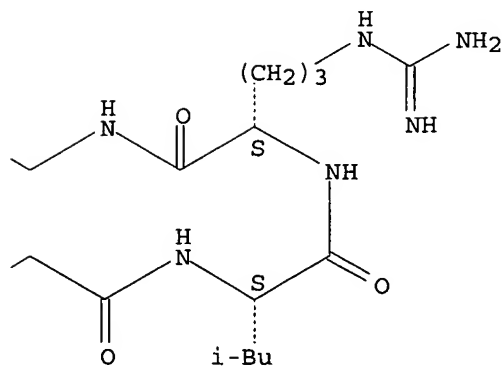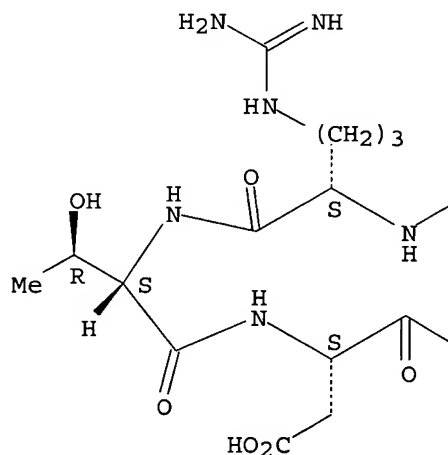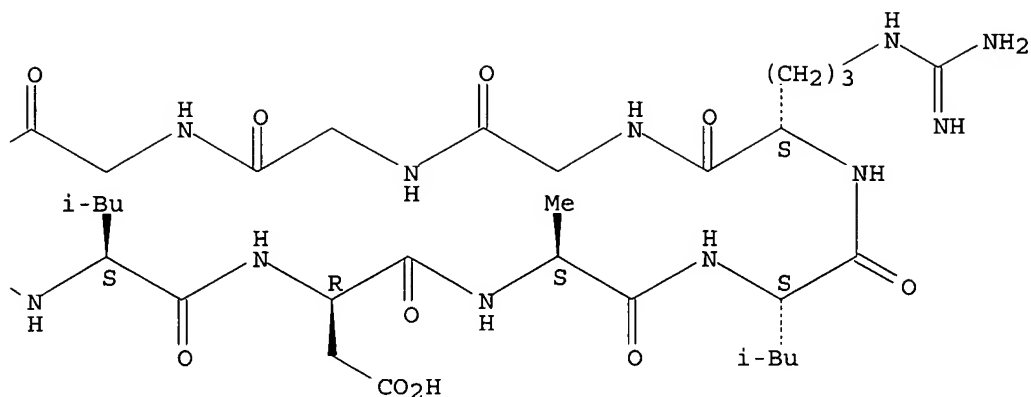RL.P   Roles from patents: BIOL (Biological study); PREP (Preparation); USES
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Absolute stereochemistry.

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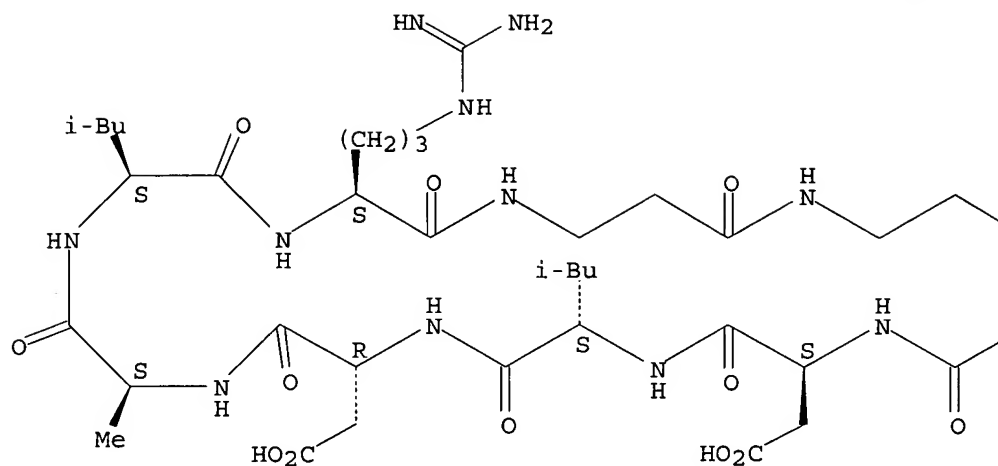
i-Bu

Me

$(CH_2)_3$—NH—C—NH$_2$, NH

NH, C, NH$_2$, $(CH_2)_3$—NH

HO$_2$C—CH$_2$

HO$_2$C—CH$_2$

i-Bu

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Absolute stereochemistry.
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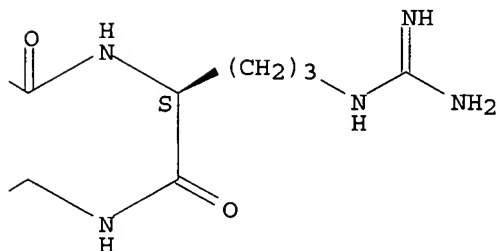
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NTE   cyclic

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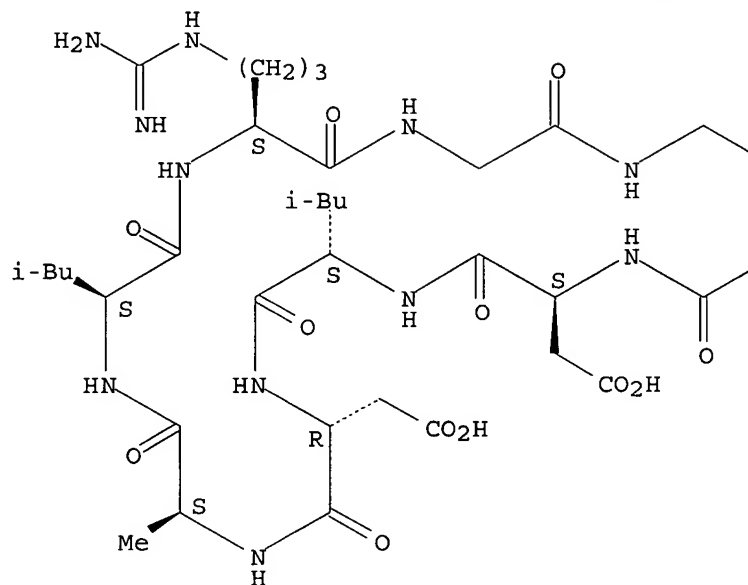
Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

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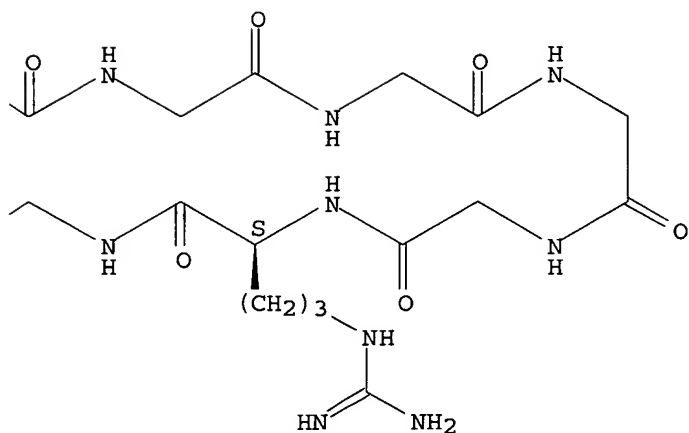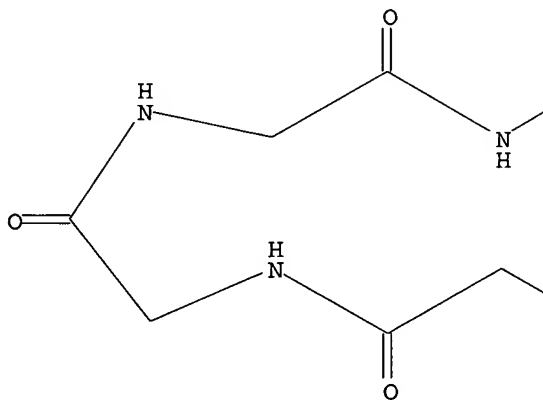MF   C45 H77 N17 O16
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DT.CA CAplus document type: Patent
RL.P   Roles from patents: BIOL (Biological study); PREP (Preparation); USES
       (Uses)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE   1: 134:86549

L3   ANSWER 17 OF 30   REGISTRY   COPYRIGHT 2005 ACS on STN
RN   317366-62-4   REGISTRY
CN   Cyclo(L-arginylglycylglycylglycyl-L-arginyl-L-threonyl-L-α-aspartyl-

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L-leucyl-D-α-aspartylglycyl-L-leucyl) (9CI)   (CA INDEX NAME)
FS   PROTEIN SEQUENCE; STEREOSEARCH
SQL   11
NTE   **cyclic**

SEQ   1 RGGGRTDLDG L
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HITS AT: 1, 5-11

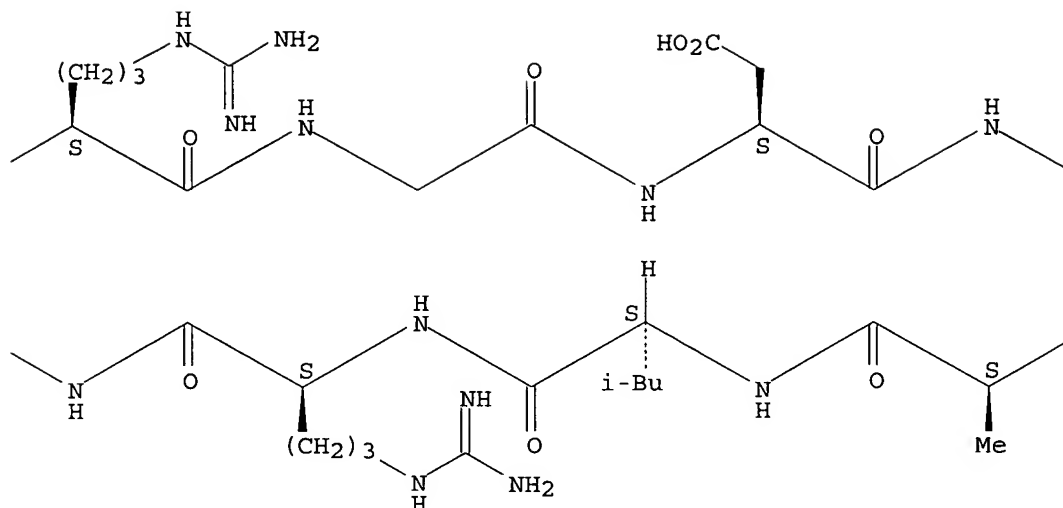**RELATED SEQUENCES AVAILABLE WITH SEQLINK**
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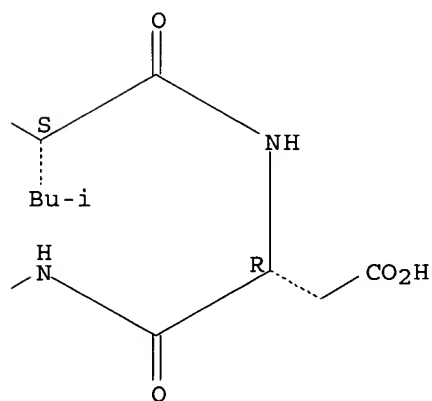   (Uses)

Absolute stereochemistry.

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PAGE 1-B

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

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REFERENCE   1:  134:86549

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RN    317366-61-3  REGISTRY
CN    Cyclo(L-alanyl-L-leucyl-L-arginylglycylglycylglycyl-L-arginyl-L-threonyl-L-
      α-aspartyl-L-leucyl-D-α-aspartyl) (9CI)  (CA INDEX NAME)
FS    PROTEIN SEQUENCE; STEREOSEARCH
SQL   11
NTE   cyclic

SEQ      1 ALRGGGRTDL D
           ===   ==== =
HITS AT:   1-3, 7-11

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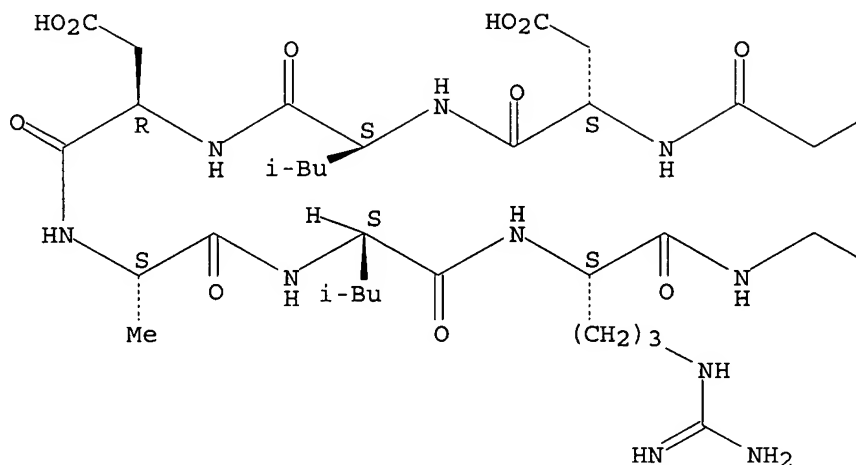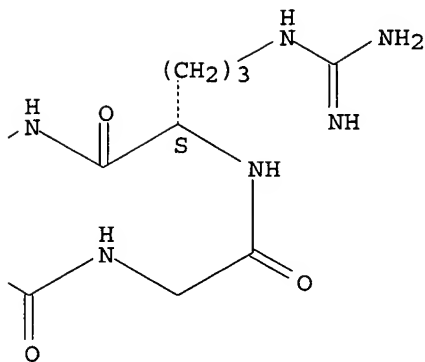
Absolute stereochemistry.

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L3     ANSWER 19 OF 30  REGISTRY  COPYRIGHT 2005 ACS on STN
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CN     Cyclo(β-alanyl-β-alanyl-L-arginylglycyl-L-α-aspartyl-L-
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       NAME)
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SQL    10
NTE    cyclic
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uncommon            Bal-5               -            -
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Absolute stereochemistry.
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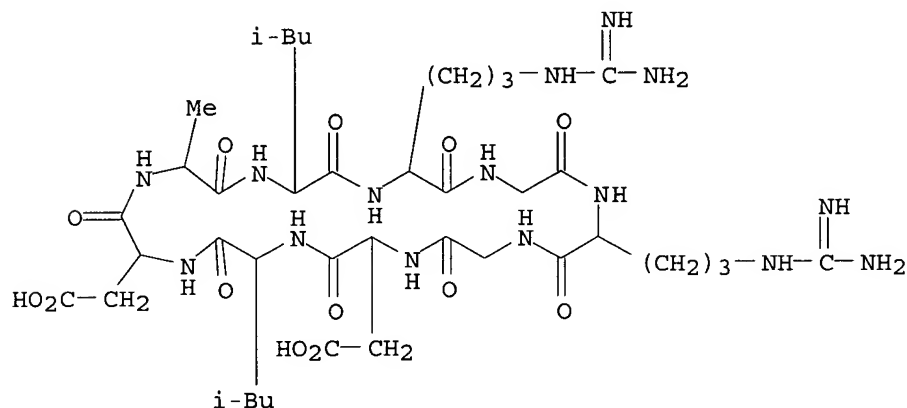
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CN    Cyclo(L-alanyl-L-leucyl-L-arginylglycylglycylglycylglycylglycylglycyl-L-
      arginylglycyl-L-α-aspartyl-L-leucyl-D-α-aspartyl) (9CI)   (CA
      INDEX NAME)
FS    PROTEIN SEQUENCE; STEREOSEARCH
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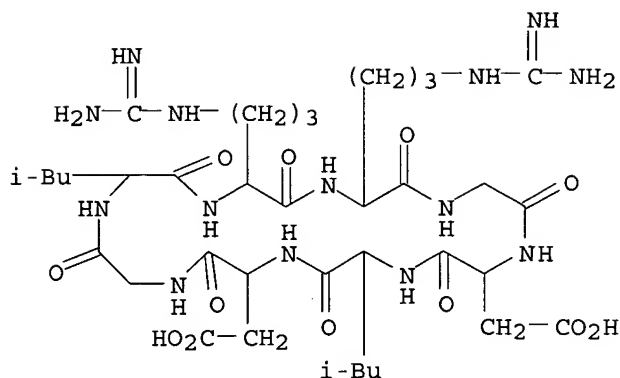
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      (Uses)

Absolute stereochemistry.

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1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE   1:   134:86549

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L3    ANSWER 21 OF 30  REGISTRY  COPYRIGHT 2005 ACS on STN
RN    317366-58-8  REGISTRY
CN    Cyclo(L-alanyl-L-leucyl-L-arginylglycylglycylglycyl-L-arginylglycyl-L-
      α-aspartyl-L-leucyl-D-α-aspartyl) (9CI)  (CA INDEX NAME)
FS    PROTEIN SEQUENCE; STEREOSEARCH
SQL   11
NTE   cyclic

SEQ      1 ALRGGGRGDL D
           ===   ==== =
HITS AT:  1-3, 7-11

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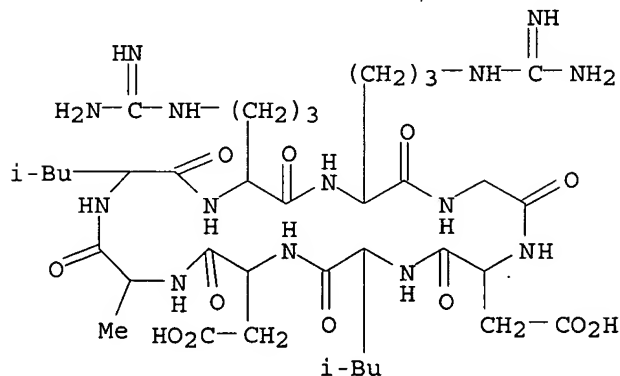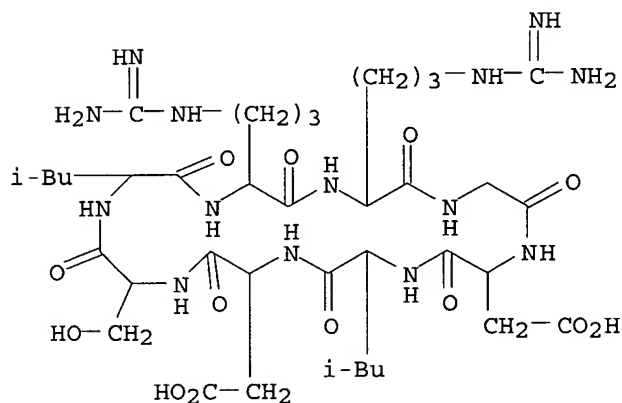
Absolute stereochemistry.

PAGE 1-A

1 REFERENCES IN FILE CA (1907 TO DATE)
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REFERENCE   1: 134:86549

L3   ANSWER 22 OF 30 REGISTRY COPYRIGHT 2005 ACS on STN
RN   317366-57-7 REGISTRY
CN   Cyclo(L-alanyl-L-leucyl-L-arginylglycylglycyl-L-arginylglycyl-L-α-
     aspartyl-L-leucyl-D-α-aspartyl) (9CI) (CA INDEX NAME)
FS   PROTEIN SEQUENCE; STEREOSEARCH
SQL 10
NTE **cyclic**

SEQ   1 ALRGGRGDLD

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HITS AT:   1-3, 6-10
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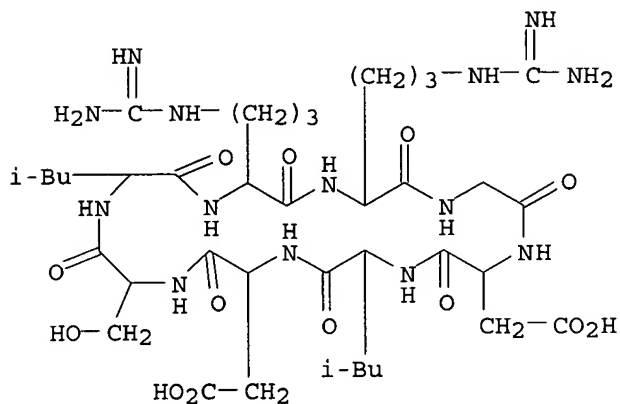
Absolute stereochemistry.

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CN    Cyclo(L-alanyl-L-leucyl-L-arginylglycyl-L-arginylglycyl-L-α-aspartyl-
      L-leucyl-D-α-aspartyl) (9CI)  (CA INDEX NAME)
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SQL   9
NTE   cyclic

SEQ        1 ALRGRGDLD
             === =====
HITS AT:    1-3, 5-9

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REFERENCE    1:  138:385705

REFERENCE    2:  134:86549


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RN    317366-54-4  REGISTRY
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NTE   cyclic

SEQ        1 RRGDLDGL
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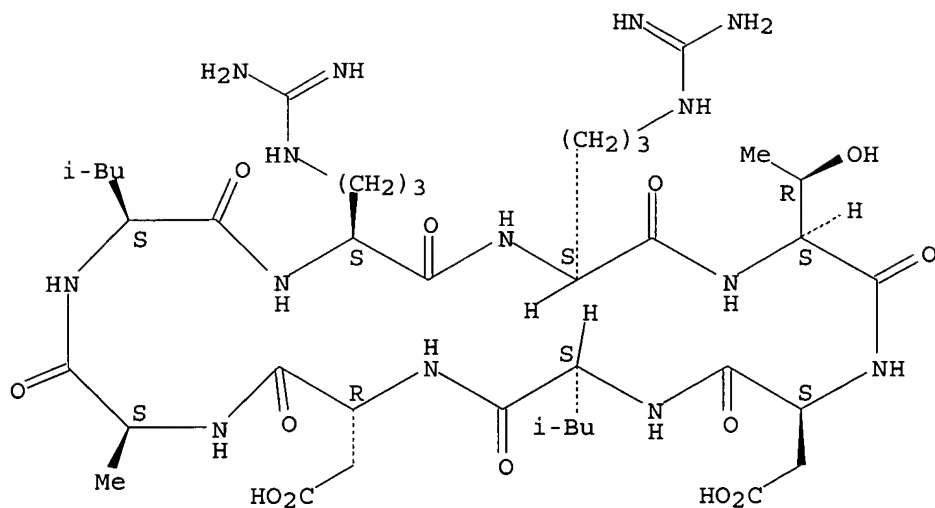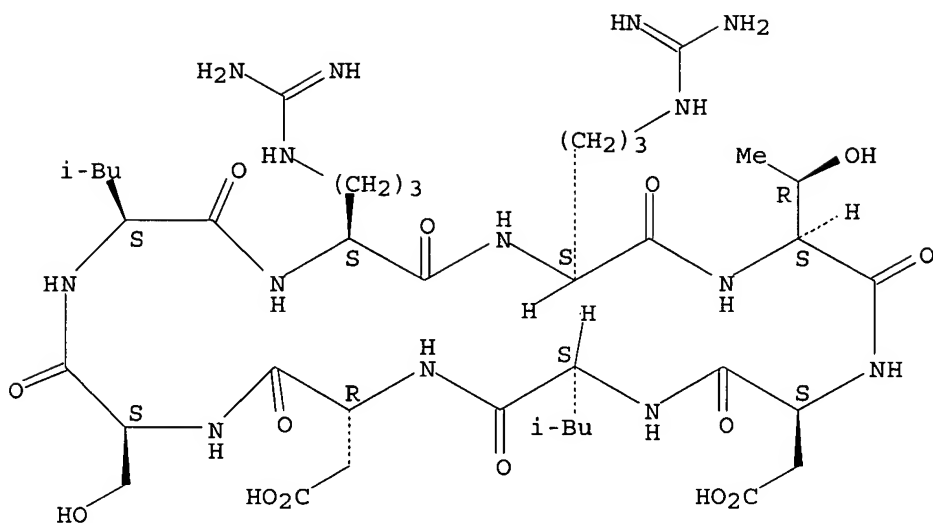
Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

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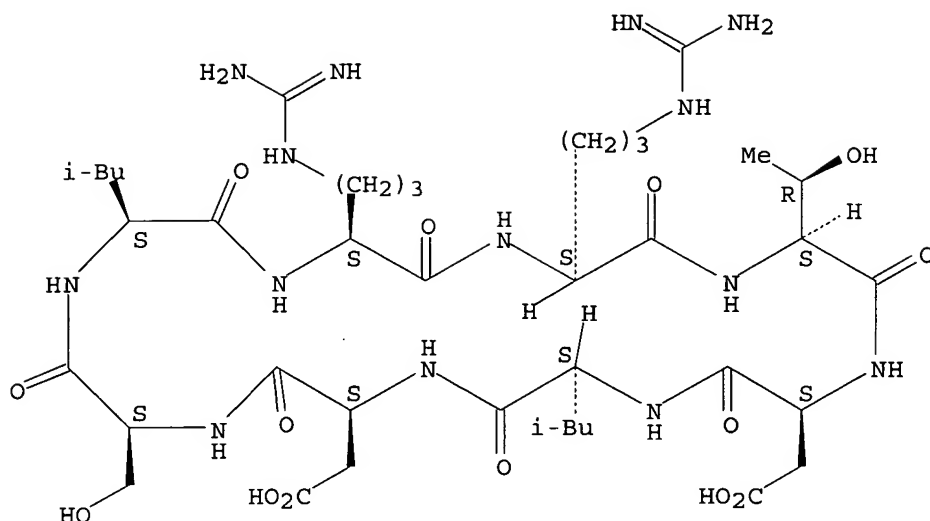

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

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REFERENCE   1:  134:86549

L3    ANSWER 26 OF 30  REGISTRY  COPYRIGHT 2005 ACS on STN
RN    317366-52-2  REGISTRY
CN    Cyclo(L-arginyl-L-arginylglycyl-L-α-aspartyl-L-leucyl-D-α-
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NTE   cyclic

SEQ      1 RRGDLDSL
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REFERENCE   1:  134:86549

L3    ANSWER 27 OF 30  REGISTRY  COPYRIGHT 2005 ACS on STN
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CN    Cyclo(L-arginyl-L-arginylglycyl-L-α-aspartyl-L-leucyl-L-α-
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FS    PROTEIN SEQUENCE; STEREOSEARCH
SQL   8
NTE   cyclic

SEQ      1 RRGDLDSL
           ========
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HITS AT: 1, 2-8

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      (Uses)

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NTE   **cyclic**

SEQ   1 ALRRTDLD
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RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES
      (Uses)

Absolute stereochemistry.

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

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REFERENCE    1:  134:86549

L3    ANSWER 29 OF 30  REGISTRY  COPYRIGHT 2005 ACS on STN
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CN    Cyclo(L-arginyl-L-arginyl-L-threonyl-L-α-aspartyl-L-leucyl-D-α-
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SEQ       1 RRTDLDSL
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Absolute stereochemistry.
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Absolute stereochemistry.

1 REFERENCES IN FILE CA (1907 TO DATE)
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REFERENCE   1:   134:86549

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=> s zischinsky g?/au;s groth u?/au;s diefenbach b?/au;s jonczyk a?/au
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L6   0 FILE EMBASE
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L12   89 FILE CAPLUS

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

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L33  ANSWER 1 OF 1  CAPLUS  COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER:        2001:45035  CAPLUS
DOCUMENT NUMBER:         134:86549
TITLE:                   Preparation of cyclic peptides for use as inhibitors
                         of integrin αvβ6
INVENTOR(S):             Jonczyk, Alfred; Diefenbach, Beate; Goodman, Simon
PATENT ASSIGNEE(S):      Merck Patent G.m.b.H., Germany
SOURCE:                  Ger. Offen., 20 pp.
                         CODEN: GWXXBX
DOCUMENT TYPE:           Patent
LANGUAGE:                German
FAMILY ACC. NUM. COUNT:  1
PATENT INFORMATION:

      PATENT NO.         KIND  DATE        APPLICATION NO.         DATE
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        WO 2001005810         A3      20010517
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                                                  WO 2000-EP6188      W    20000703
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      Ser; X5 = Leu, Ile, Nle, Val, Phe; X6 = Arg, Har, Lys; R1 = absent, one or
      more ω-amino-carboxy acid residues; all amino acids may be either D-
      or L-configuration] were prepared using solid-phase peptide synthesis and
      tested for activity as integrin αvβ6 inhibitors for therapeutic
      use.  Thus thirty-three I compds. were synthesized on chlorotrityl-
      polystyrol resin and tested for their binding capacities with the
      αvβ6 fibronectin receptor.  Q-values for the tests (Q = IC50
      I/IC50 reference peptide) (reference peptide =
Ac-Arg-Thr-Asp-Leu-Asp-Ser-Leu-Arg-
      NH2; 75 nM) ranged from 233 to 0.014.
IT    317366-48-6P 317366-49-7P 317366-50-0P
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      study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
      BIOL (Biological study); PREP (Preparation); USES (Uses)
          (preparation of cyclic peptides for use as inhibitors of integrin
          αvβ6 in treatment of)
RN    317366-48-6  CAPLUS
CN    Cyclo(L-arginyl-L-arginyl-L-threonyl-L-α-aspartyl-L-leucyl-L-α-
      aspartyl-L-seryl-L-leucyl) (9CI)   (CA INDEX NAME)

NTE   cyclic

SEQ      1 RRTDLDSL
```

Absolute stereochemistry.

RN   317366-49-7   CAPLUS
CN   Cyclo(L-arginyl-L-arginyl-L-threonyl-L-α-aspartyl-L-leucyl-D-α-
      aspartyl-L-seryl-L-leucyl) (9CI)   (CA INDEX NAME)

NTE   cyclic

SEQ   1 RRTDLDSL

Absolute stereochemistry.
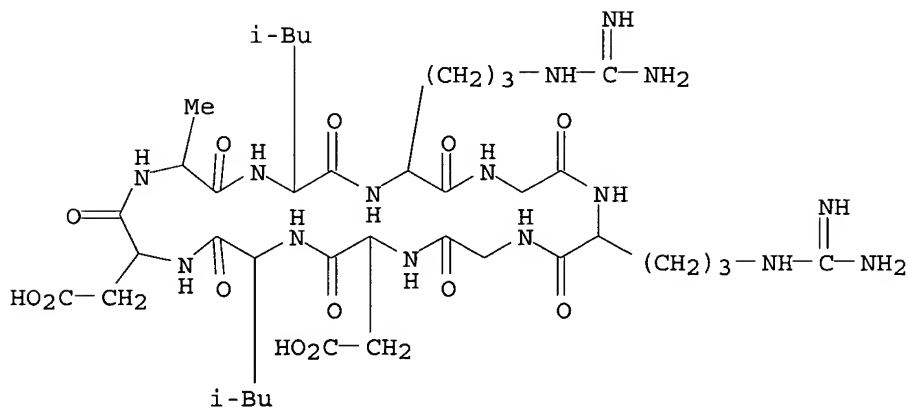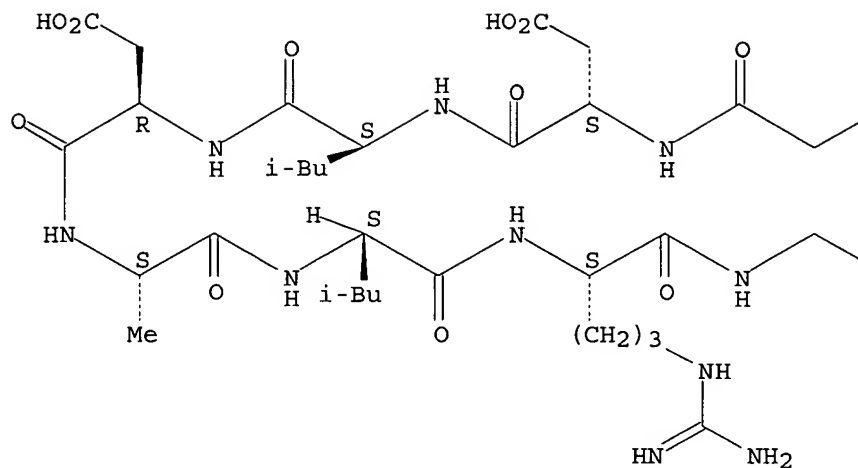

RN   317366-50-0   CAPLUS
CN   Cyclo(L-alanyl-L-leucyl-L-arginyl-L-arginyl-L-threonyl-L-α-aspartyl-
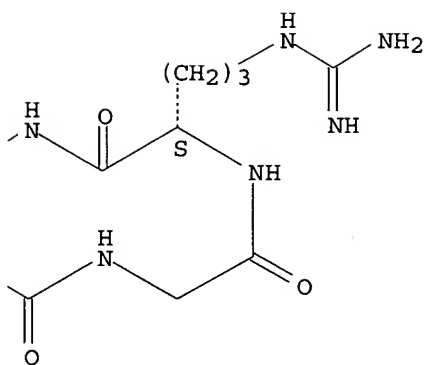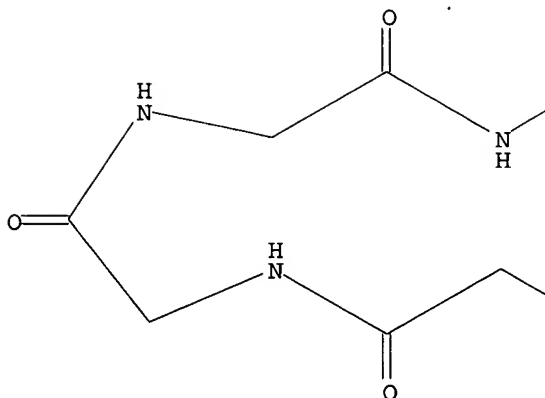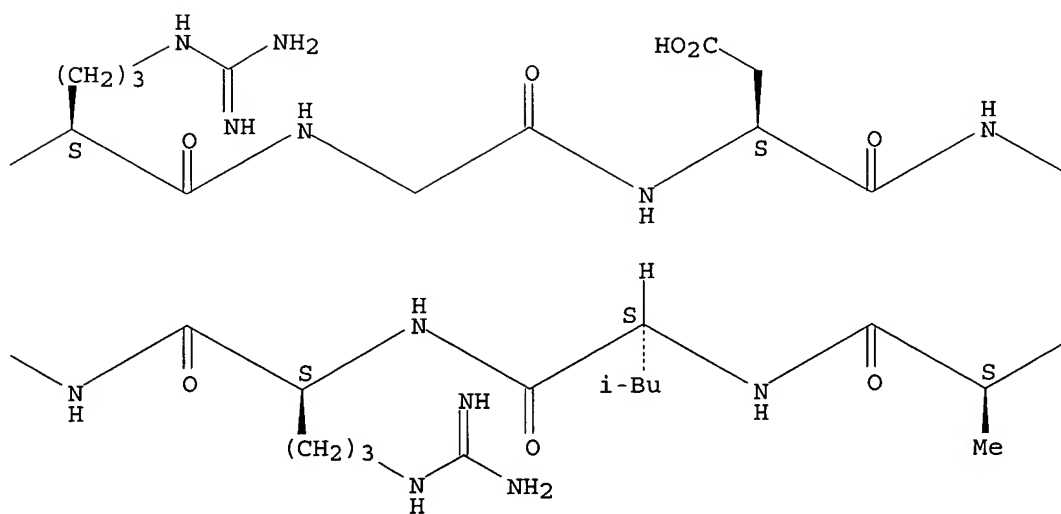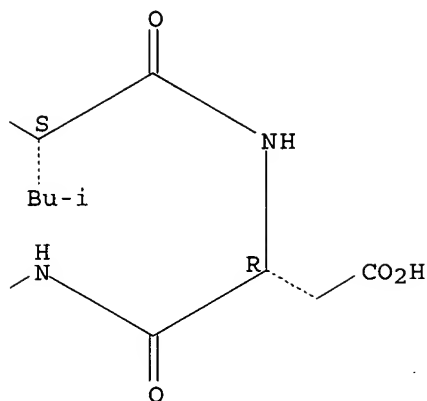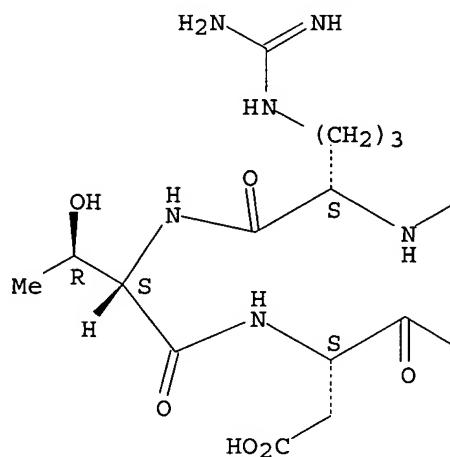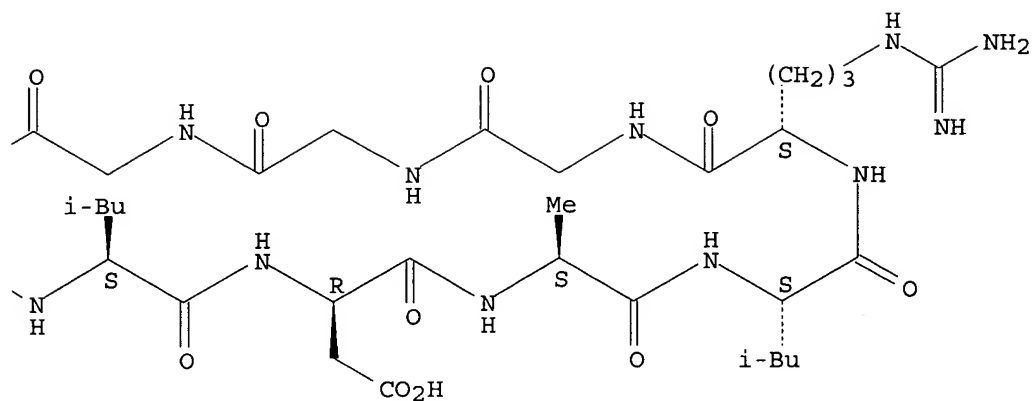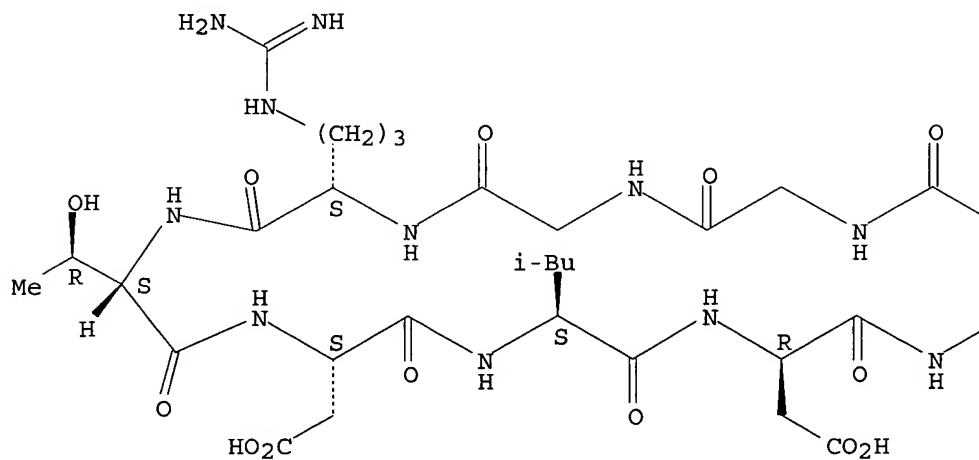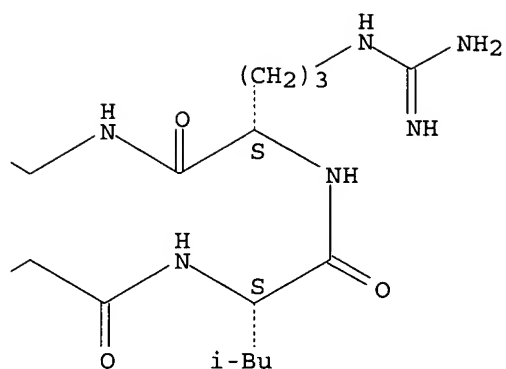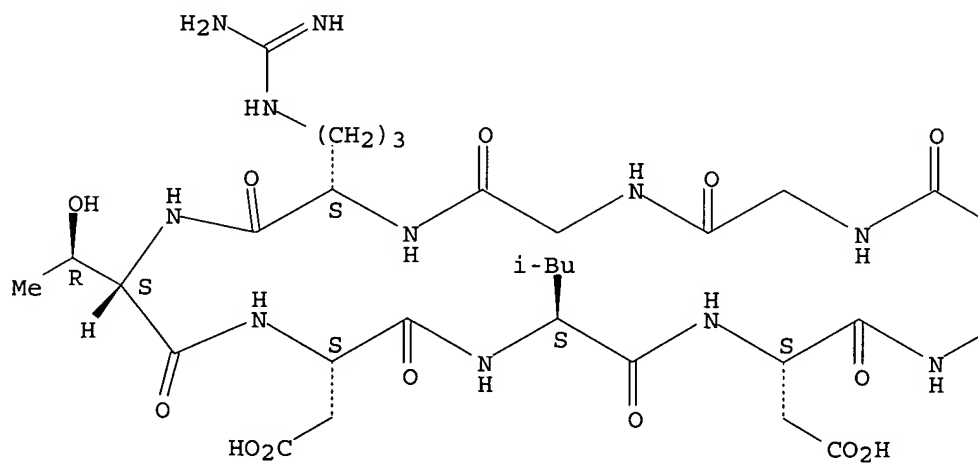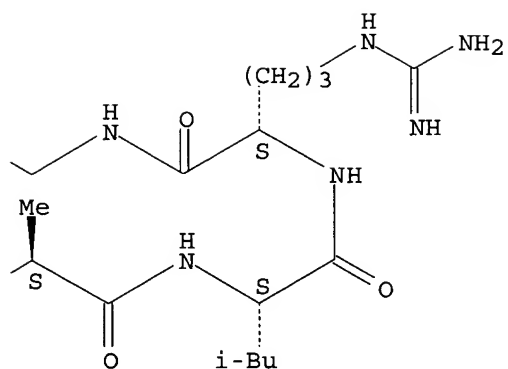   L-leucyl-D-α-aspartyl) (9CI)   (CA INDEX NAME)
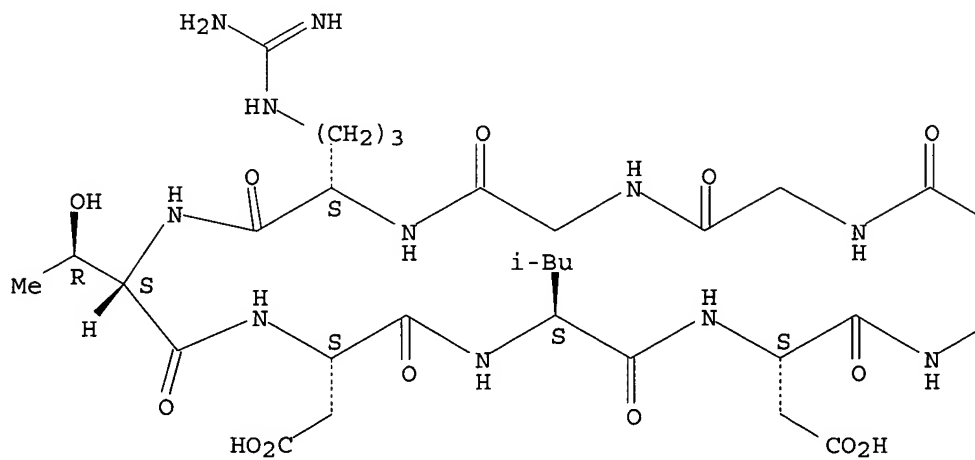
NTE   cyclic

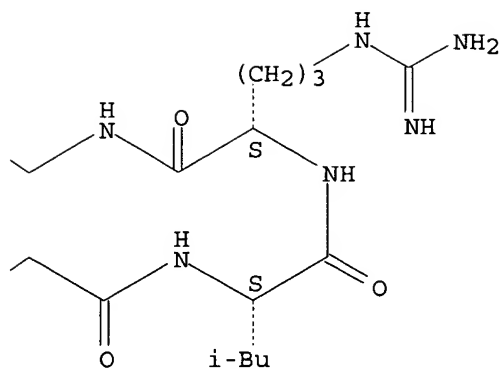SEQ 1 ALRRTDLD

Absolute stereochemistry.

RN 317366-51-1 CAPLUS
CN Cyclo(L-arginyl-L-arginylglycyl-L-α-aspartyl-L-leucyl-L-α-aspartyl-L-seryl-L-leucyl) (9CI) (CA INDEX NAME)

NTE cyclic

SEQ 1 RRGDLDSL

RN 317366-52-2 CAPLUS
CN Cyclo(L-arginyl-L-arginylglycyl-L-α-aspartyl-L-leucyl-D-α-aspartyl-L-seryl-L-leucyl) (9CI) (CA INDEX NAME)

NTE cyclic

SEQ 1 RRGDLDSL

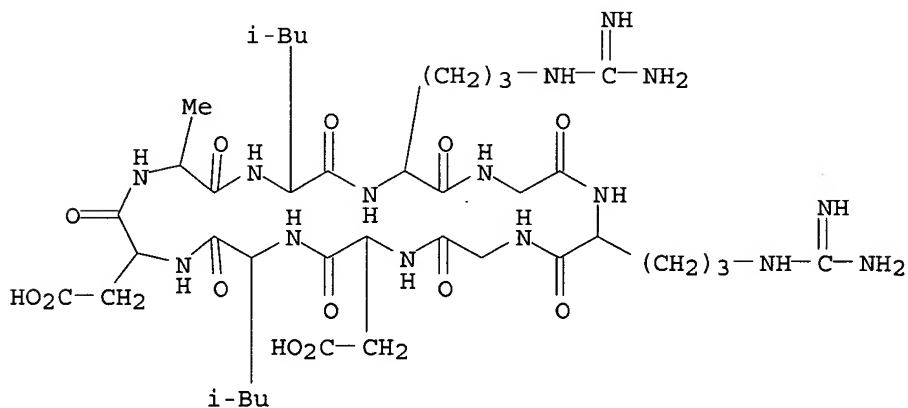Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

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RN   317366-53-3   CAPLUS
CN   Cyclo(L-alanyl-L-leucyl-L-arginyl-L-arginylglycyl-L-α-aspartyl-L-
      leucyl-D-α-aspartyl) (9CI)   (CA INDEX NAME)

NTE   cyclic

SEQ   1 ALRRGDLD

RN   317366-54-4   CAPLUS
CN   Cyclo(L-arginyl-L-arginylglycyl-L-α-aspartyl-L-leucyl-D-α-
      aspartylglycyl-L-leucyl) (9CI)   (CA INDEX NAME)

NTE   cyclic

SEQ   1 RRGDLDGL

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RN   317366-56-6   CAPLUS
CN   Cyclo(L-alanyl-L-leucyl-L-arginylglycyl-L-arginylglycyl-L-α-aspartyl-
      L-leucyl-D-α-aspartyl) (9CI)   (CA INDEX NAME)

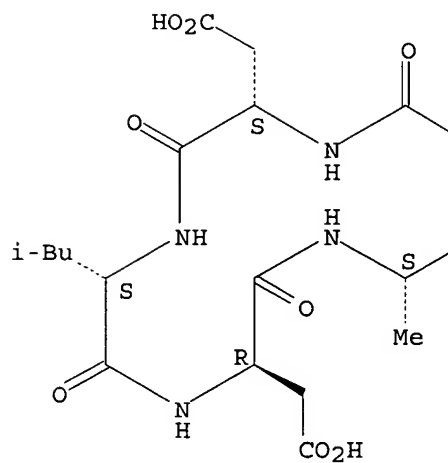NTE   cyclic

SEQ   1 ALRGRGDLD

RN   317366-57-7   CAPLUS
CN   Cyclo(L-alanyl-L-leucyl-L-arginylglycylglycyl-L-arginylglycyl-L-α-
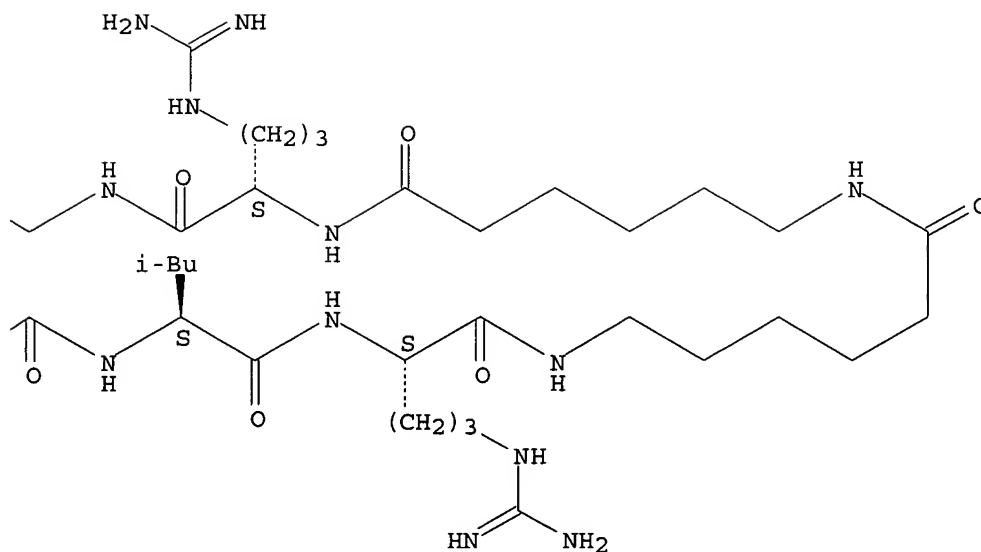   aspartyl-L-leucyl-D-α-aspartyl) (9CI)   (CA INDEX NAME)

NTE   cyclic

SEQ   1 ALRGGRGDLD

Absolute stereochemistry.

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RN   317366-58-8   CAPLUS
CN   Cyclo(L-alanyl-L-leucyl-L-arginylglycylglycylglycyl-L-arginylglycyl-L-
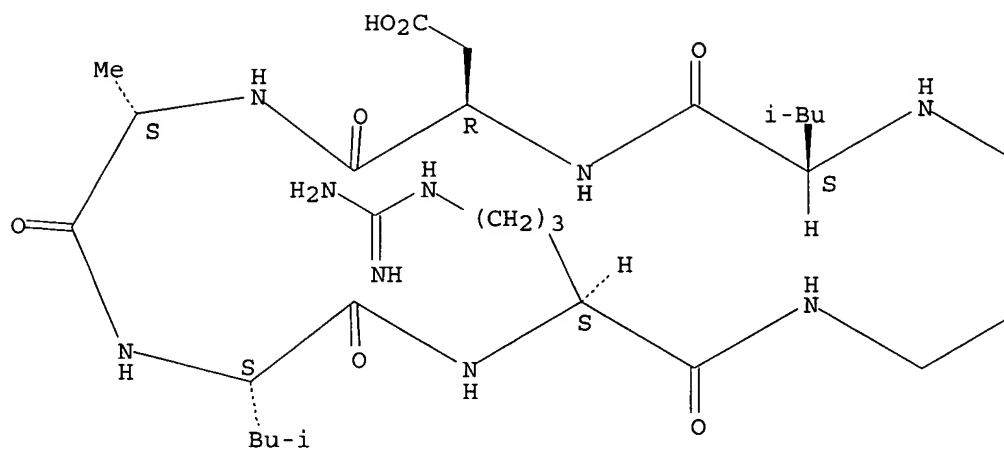   α-aspartyl-L-leucyl-D-α-aspartyl) (9CI)   (CA INDEX NAME)
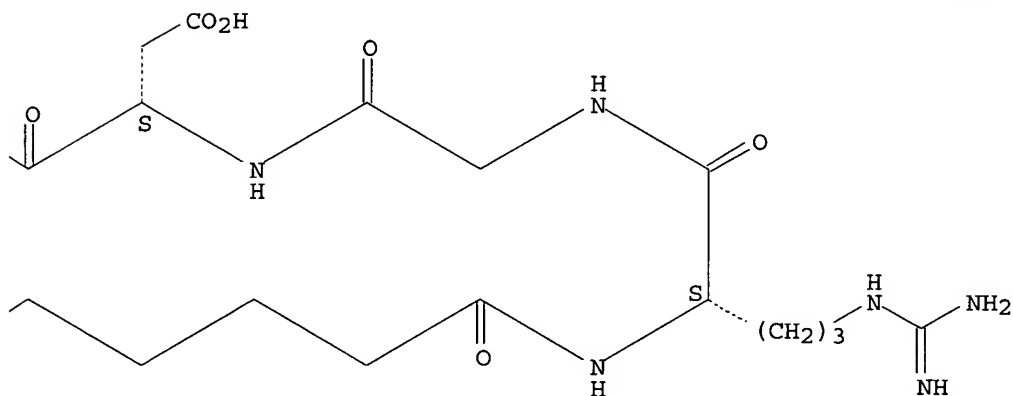
NTE   cyclic

SEQ   1 ALRGGGRGDL D

Absolute stereochemistry.

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RN   317366-59-9   CAPLUS
CN   Cyclo(L-alanyl-L-leucyl-L-arginylglycylglycylglycylglycylglycylglycyl-L-
      arginylglycyl-L-α-aspartyl-L-leucyl-D-α-aspartyl) (9CI)   (CA
      INDEX NAME)

NTE   cyclic

SEQ   1 ALRGGGGGGR GDLD

Absolute stereochemistry.

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RN 317366-60-2 CAPLUS
CN Cyclo(β-alanyl-β-alanyl-L-arginylglycyl-L-α-aspartyl-L-
leucyl-D-α-aspartyl-L-alanyl-L-leucyl-L-arginyl) (9CI) (CA INDEX
NAME)

NTE cyclic

SEQ 1 ALRXXRGDLD

Absolute stereochemistry.

PAGE 1-A

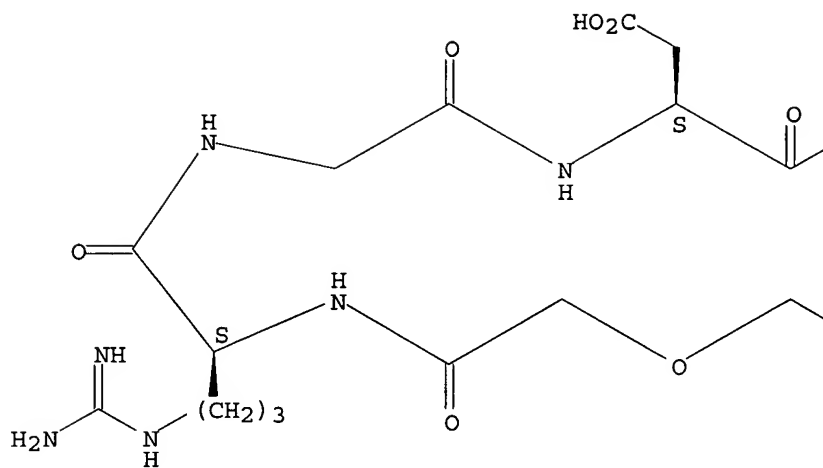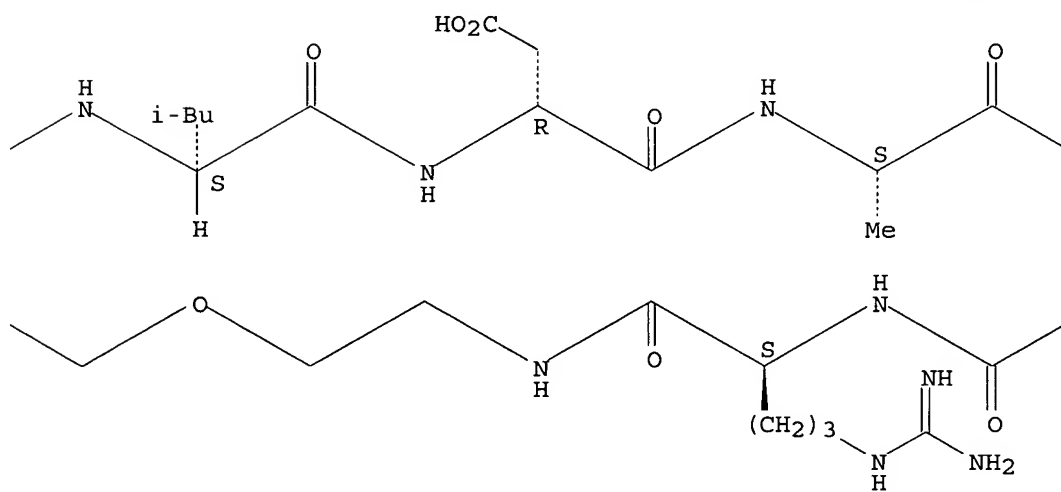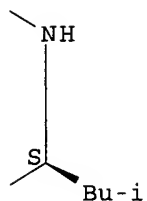Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

RN   317366-61-3   CAPLUS
CN   Cyclo(L-alanyl-L-leucyl-L-arginylglycylglycylglycyl-L-arginyl-L-threonyl-L-
     α-aspartyl-L-leucyl-D-α-aspartyl) (9CI)   (CA INDEX NAME)

NTE cyclic

SEQ   1 ALRGGGRTDL D

Absolute stereochemistry.

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RN   317366-62-4   CAPLUS
CN   Cyclo(L-arginylglycylglycylglycyl-L-arginyl-L-threonyl-L-α-aspartyl-
      L-leucyl-D-α-aspartylglycyl-L-leucyl) (9CI)   (CA INDEX NAME)

NTE   cyclic

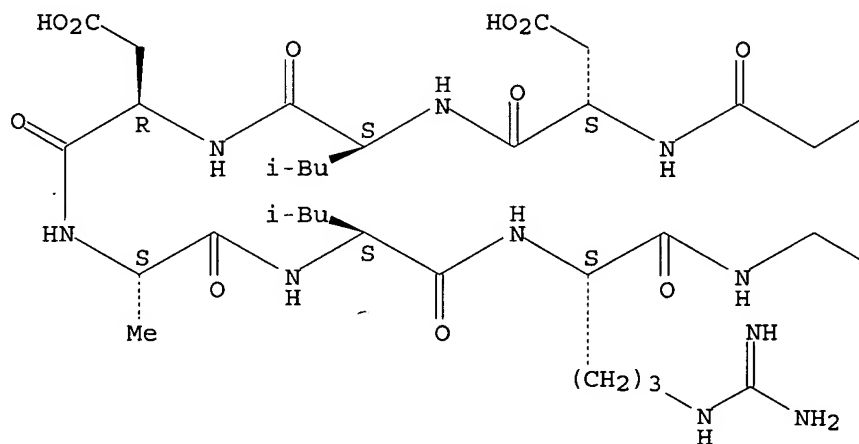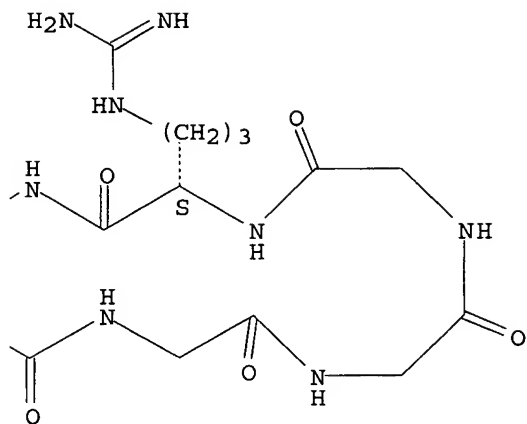SEQ   1 RGGGRTDLDG L

Absolute stereochemistry.

RN   317366-63-5   CAPLUS
CN   Cyclo(L-alanyl-L-leucyl-L-arginylglycylglycylglycyl-L-arginyl-L-threonyl-L-
      α-aspartyl-L-leucyl-L-α-aspartyl) (9CI)   (CA INDEX NAME)

NTE   cyclic

SEQ   1 ALRGGGRTDL D
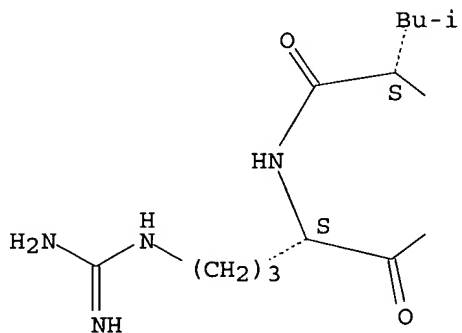

Absolute stereochemistry.

RN   317366-64-6 CAPLUS
CN   Cyclo(L-arginylglycylglycylglycyl-L-arginyl-L-threonyl-L-α-aspartyl-
      L-leucyl-L-α-aspartylglycyl-L-leucyl) (9CI)   (CA INDEX NAME)

NTE   cyclic

SEQ   1 RGGGRTDLDG L

Absolute stereochemistry.

H
N—NH₂
(CH₂)3
NH

H
N   O
S
NH

H
N
S
O

O
i-Bu

RN   317366-65-7   CAPLUS
CN   Cyclo(L-alanyl-L-leucyl-L-arginylglycyl-L-arginylglycyl-L-α-aspartyl-
      L-leucyl-L-α-aspartyl) (9CI)   (CA INDEX NAME)

NTE   cyclic
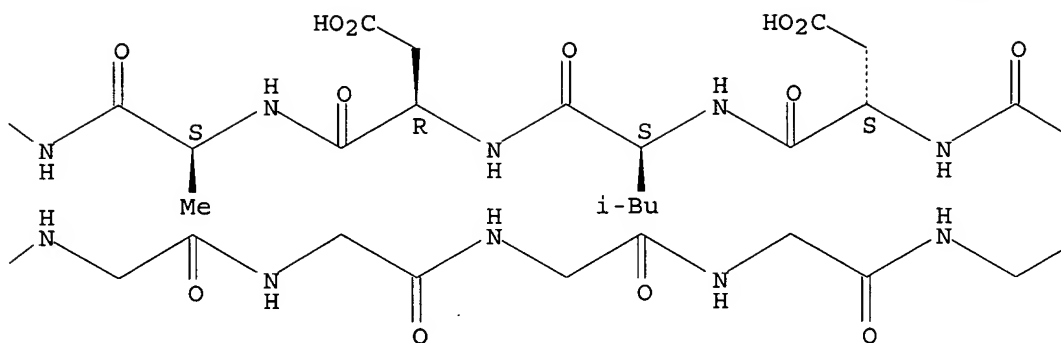
SEQ   1 ALRGRGDLD

i-Bu
Me
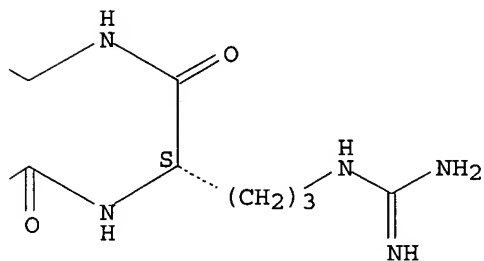NH
(CH₂)3—NH—C—NH₂

H   O H   O H
N   N   N   O
O   NH
NH   NH   NH
H   H   H
HO₂C—CH₂   O   O   O   O   (CH₂)3—NH—C—NH₂
HO₂C—CH₂   NH
i-Bu

RN   317366-68-0   CAPLUS
CN   Cyclo(L-alanyl-L-leucyl-L-arginyl-6-aminohexanoyl-6-aminohexanoyl-L-
      arginylglycyl-L-α-aspartyl-L-leucyl-D-α-aspartyl) (9CI)   (CA
      INDEX NAME)

NTE   cyclic

SEQ   1 ALRXXRGDLD
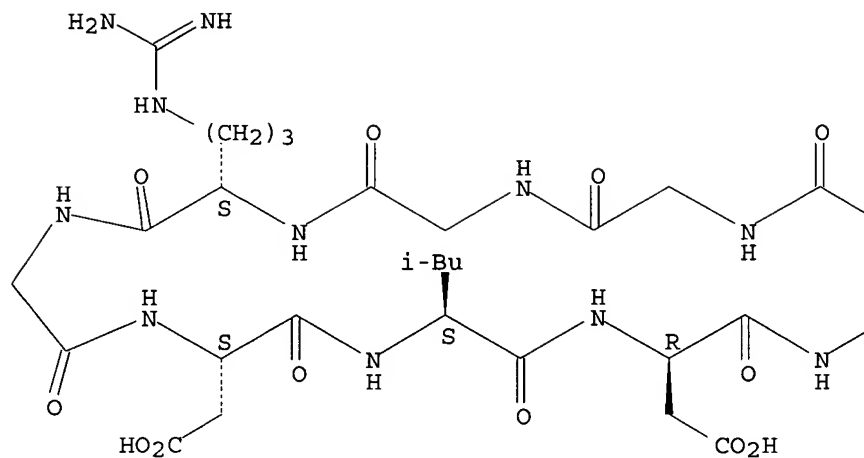

Absolute stereochemistry.

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PAGE 1-B

NTE   cyclic

SEQ   1 ALRXRGDLD

Absolute stereochemistry.

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```
RN    317366-70-4  CAPLUS
CN    Cyclo[[2-(2-aminoethoxy)ethoxy]acetyl-L-arginylglycyl-L-α-aspartyl-L-
      leucyl-D-α-aspartyl-L-alanyl-L-leucyl-L-arginyl] (9CI)  (CA INDEX
      NAME)

NTE   cyclic

SEQ      1 ALRXRGDLD
```

Absolute stereochemistry.

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Prepared by: Mary Hale @2-2507 Rem Bldg 1D86
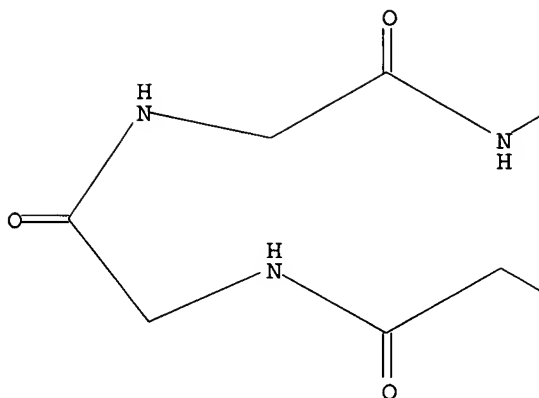
NH

S

Bu-i

RN   317366-71-5   CAPLUS
CN   Cyclo(L-alanyl-L-leucyl-L-arginylglycylglycylglycylglycyl-L-arginylglycyl-
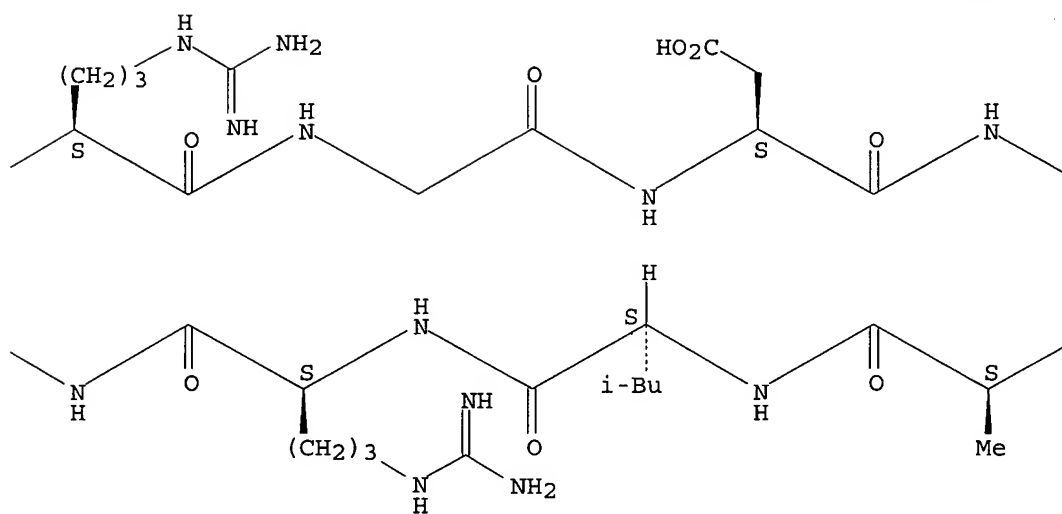   L-α-aspartyl-L-leucyl-D-α-aspartyl) (9CI)   (CA INDEX NAME)
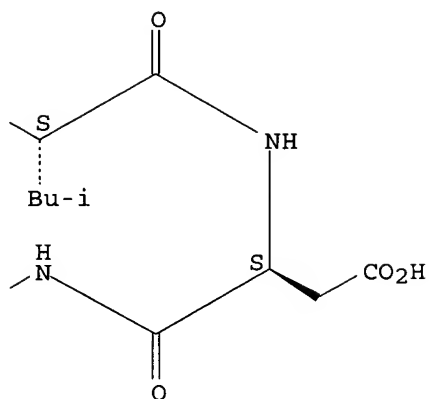
NTE   cyclic

SEQ   1 ALRGGGGRGD LD

Absolute stereochemistry.

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RN   317366-72-6   CAPLUS
CN   Cyclo(L-alanyl-L-leucyl-L-arginylglycylglycylglycylglycylglycyl-L-
       arginylglycyl-L-α-aspartyl-L-leucyl-D-α-aspartyl) (9CI)   (CA
       INDEX NAME)

NTE   cyclic

SEQ   1 ALRGGGGGRG DLD
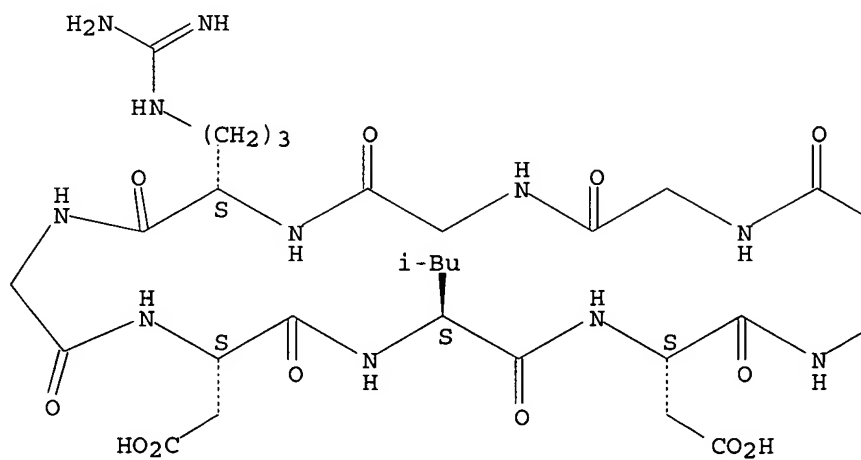

Absolute stereochemistry.

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PAGE 1-C

RN   317366-73-7 CAPLUS
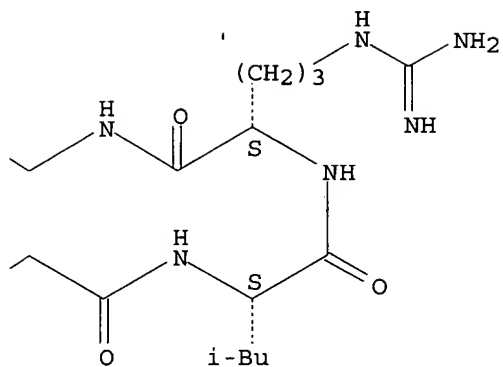CN   Cyclo(L-arginylglycyl-L-α-aspartyl-L-leucyl-D-α-aspartylglycyl-
      L-leucyl-L-arginylglycylglycylglycyl) (9CI) (CA INDEX NAME)

NTE   cyclic

SEQ   1 RGDLDGLRGG G

Absolute stereochemistry.

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RN   317366-74-8 CAPLUS
CN   Cyclo(L-alanyl-L-leucyl-L-arginylglycylglycylglycyl-L-arginylglycyl-L-
      α-aspartyl-L-leucyl-L-α-aspartyl) (9CI) (CA INDEX NAME)

NTE   cyclic

SEQ   1 ALRGGGRGDL D

Absolute stereochemistry.

RN   317366-75-9   CAPLUS

CN   Cyclo(L-arginylglycyl-L-α-aspartyl-L-leucyl-L-α-aspartylglycyl-
      L-leucyl-L-arginylglycylglycylglycyl) (9CI)   (CA INDEX NAME)

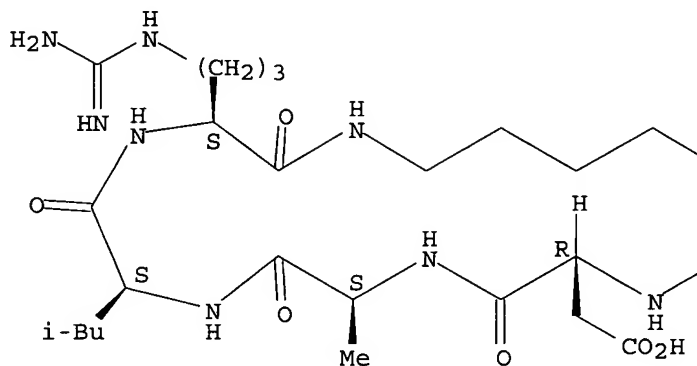NTE   cyclic

SEQ   1 RGDLDGLRGG G

Absolute stereochemistry.

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RN   317366-76-0   CAPLUS
CN   Cyclo(L-alanyl-L-leucyl-L-arginyl-6-aminohexanoyl-L-arginyl-L-threonyl-L-
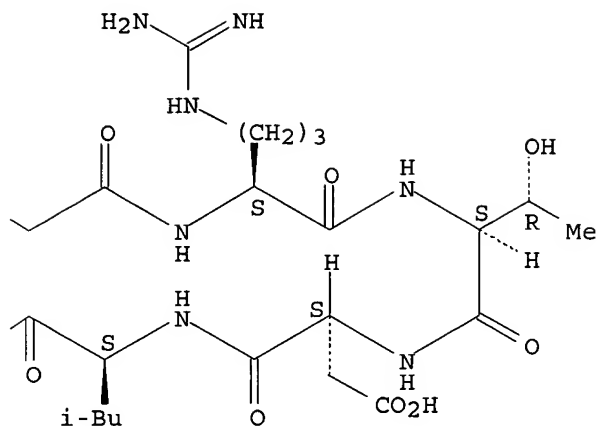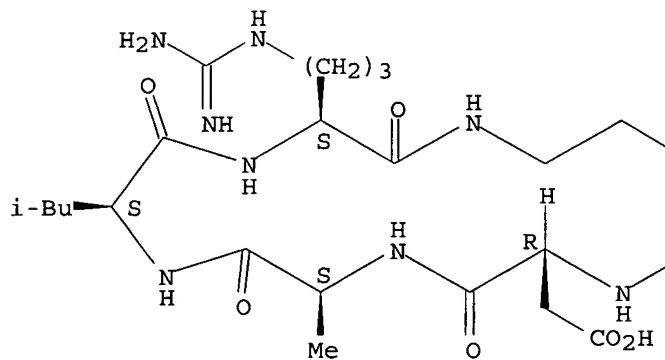   α-aspartyl-L-leucyl-D-α-aspartyl) (9CI)   (CA INDEX NAME)

NTE   cyclic

SEQ   1 ALRXRTDLD

Absolute stereochemistry.

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RN   317366-77-1 CAPLUS
CN   Cyclo(L-alanyl-L-leucyl-L-arginyl-4-aminobutanoyl-L-arginyl-L-threonyl-L-
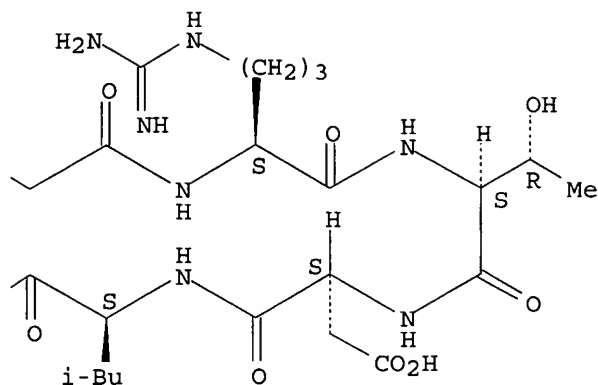α-aspartyl-L-leucyl-D-α-aspartyl) (9CI) (CA INDEX NAME)

NTE   cyclic

SEQ   1 ALRXRTDLD
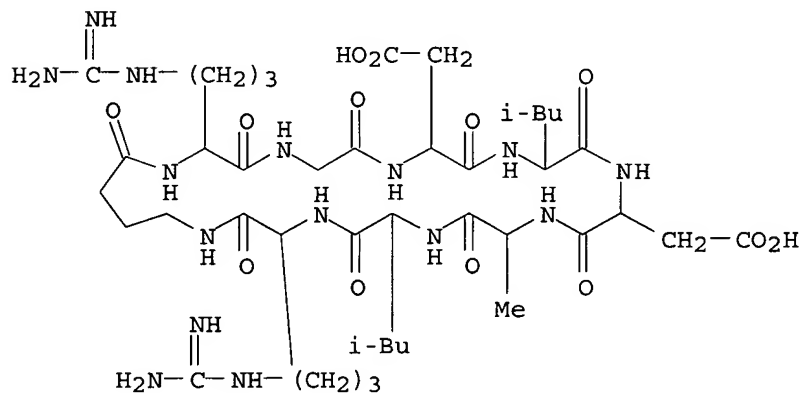

Absolute stereochemistry.

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RN   317366-78-2 CAPLUS
CN   Cyclo(L-alanyl-L-leucyl-L-arginyl-4-aminobutanoyl-L-arginylglycyl-L-
      α-aspartyl-L-leucyl-D-α-aspartyl) (9CI) (CA INDEX NAME)

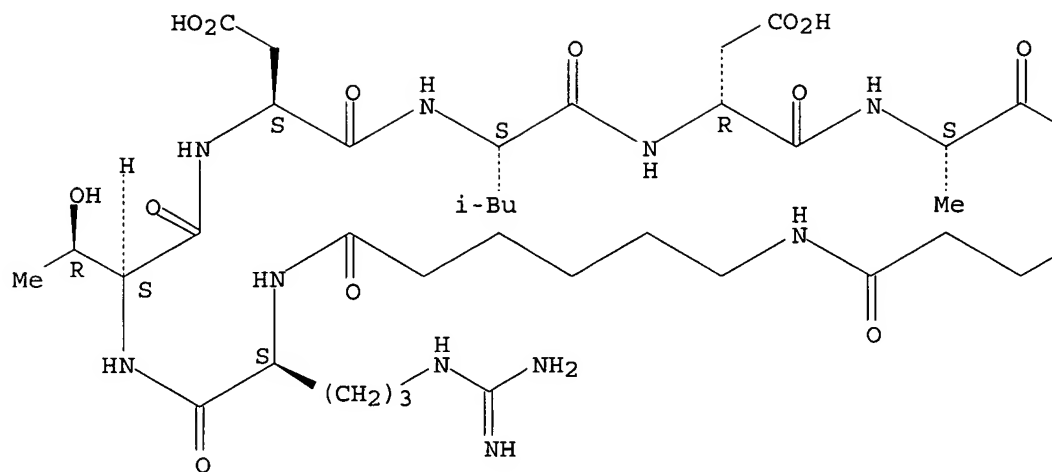NTE   cyclic

SEQ   1 ALRXRGDLD

RN   317366-79-3 CAPLUS
CN   Cyclo(L-alanyl-L-leucyl-L-arginyl-6-aminohexanoyl-6-aminohexanoyl-L-
      arginyl-L-threonyl-L-α-aspartyl-L-leucyl-D-α-aspartyl) (9CI)
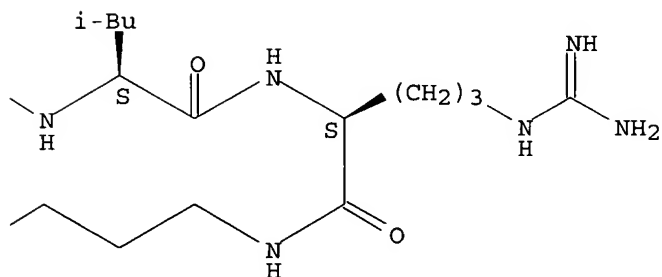   (CA INDEX NAME)

NTE   cyclic

SEQ   1 ALRXXRTDLD

Absolute stereochemistry.

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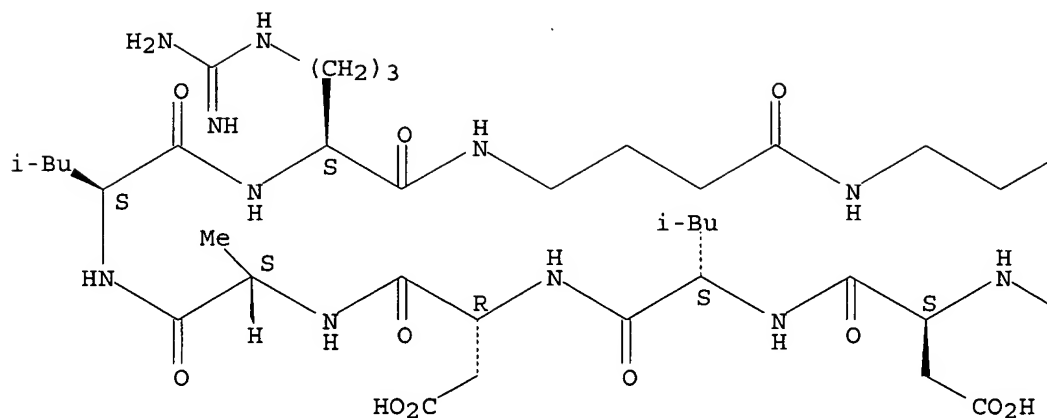
PAGE 1-A

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```
RN    317366-80-6   CAPLUS
CN    Cyclo(L-alanyl-L-leucyl-L-arginyl-4-aminobutanoyl-4-aminobutanoyl-L-
      arginyl-L-threonyl-L-α-aspartyl-L-leucyl-D-α-aspartyl) (9CI)
      (CA INDEX NAME)

NTE   cyclic

SEQ      1 ALRXXRTDLD
```
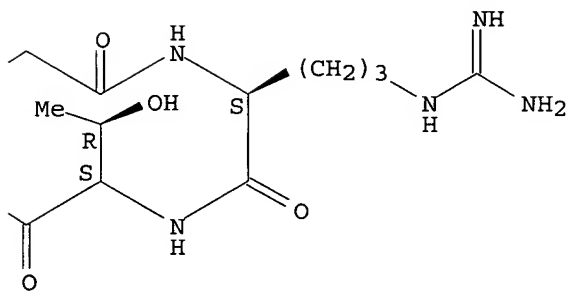
Absolute stereochemistry.

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```
=> s l3 not (l8 or l13 or l18 or l23)
L34          0 FILE MEDLINE
L35          0 FILE BIOSIS
L36          0 FILE EMBASE
L37          0 FILE CAPLUS

TOTAL FOR ALL FILES
L38          0 L3 NOT (L8 OR L13 OR L18 OR L23)

=> dis his

     (FILE 'HOME' ENTERED AT 08:31:16 ON 30 NOV 2005)

     FILE 'REGISTRY' ENTERED AT 08:31:25 ON 30 NOV 2005
L1         296 S R[SGT]D[LIXVF][DEKF][GAS][LIXVF][RXK]/SQSP
L2       27096 S CYCLIC/NTE
L3          30 S L1 AND L2

     FILE 'MEDLINE, BIOSIS, EMBASE, CAPLUS' ENTERED AT 08:33:23 ON 30 NOV 2005


Prepared by: Mary Hale @2-2507 Rem Bldg 1D86
```

```
L4              0 FILE MEDLINE
L5              0 FILE BIOSIS
L6              0 FILE EMBASE
L7              8 FILE CAPLUS
     TOTAL FOR ALL FILES
L8              8 S ZISCHINSKY G?/AU
L9             28 FILE MEDLINE
L10            56 FILE BIOSIS
L11            33 FILE EMBASE
L12            89 FILE CAPLUS
     TOTAL FOR ALL FILES
L13           206 S GROTH U?/AU
L14            10 FILE MEDLINE
L15            22 FILE BIOSIS
L16             9 FILE EMBASE
L17            44 FILE CAPLUS
     TOTAL FOR ALL FILES
L18            85 S DIEFENBACH B?/AU
L19            34 FILE MEDLINE
L20            71 FILE BIOSIS
L21            72 FILE EMBASE
L22           270 FILE CAPLUS
     TOTAL FOR ALL FILES
L23           447 S JONCZYK A?/AU
L24             0 FILE MEDLINE
L25             0 FILE BIOSIS
L26             0 FILE EMBASE
L27             4 FILE CAPLUS
     TOTAL FOR ALL FILES
L28             4 S L8 AND L13 AND L18 AND L23
L29             0 FILE MEDLINE
L30             0 FILE BIOSIS
L31             0 FILE EMBASE
L32             1 FILE CAPLUS
     TOTAL FOR ALL FILES
L33             1 S L3 NOT L28
L34             0 FILE MEDLINE
L35             0 FILE BIOSIS
L36             0 FILE EMBASE
L37             0 FILE CAPLUS
     TOTAL FOR ALL FILES
L38             0 S L3 NOT (L8 OR L13 OR L18 OR L23)

=> log y
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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	24.08	249.08

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.73	-0.73

STN INTERNATIONAL LOGOFF AT 08:36:47 ON 30 NOV 2005

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86